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The effectiveness of life cycle inventories: Conceptual data versus site-specific data.

Faiza Iskandar Abdulrahem
University of Windsor

The Effectiveness of Life Cycle Inventories: Conceptual Data versus Site-Specific Data

by

Faiza Iskandar Abdulrahem

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Abstract

Conducting a life cycle inventory (LCI) is the first step in carrying out a life cycle analysis (LCA). However, life cycle inventories are often based on surrogate or generic data because site specific data from the facility, product, or process in question does not yet exist or cannot be measured. This thesis investigates the effects of using different types of data on the credibility of life cycle inventories, and evaluates differences that exist between using site-specific data and conceptual sources of data. In particular, the thesis examines if a life cycle inventory developed by assuming data from external sources for an industrial process is reasonably comparable to a life cycle inventory using site-specific data for this same process: the former scenario is the situation most LCA practitioners find themselves in.

The pre-treatment process for automotive painting is used as a case study. Two sources of data are used to develop the life cycle inventories in this thesis: one facility provides the actual or site specific data, while a second facility provides the surrogate data that will be used to model the process. Both facilities have similar but not identical processes. The thesis also considers other sources for data that are frequently used by LCA practitioners if site-specific data is missing or incomplete, such as the online sources, industry literature, and government or industry databases. The results from the surrogate data versus site-specific data derived LCIs were examined, as well as the differences among all the different types of data, and the quality of the data acquired.

Differences were found to exist in all levels of the inventory starting with the products used, their constituents, and concentrations and ending with the type of reported emissions. Furthermore, there did not appear to be a uniform correction factor that LCA practitioners could apply to adjust for using conceptual rather than process or site specific data. However, not all results were found to be equally sensitive to changes in the data variables and that the differences, while significant, may be acceptable for LCIs depending on the purpose of the LCI study.

Dedication

In the name of Allah,

Most Gracious, Most Merciful

This work is dedicated

To

My beloved, supportive husband **Ayyad ♥,**

Wonderful, forbearing children **Dalia♥** and **Ibraheem♥,**

My dearest parents and family

Also dedicated to

Everyone who contributed to this work with sincere, good intention

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Chapter 1: The Role of Life Cycle Inventories

The increasing awareness of the importance of assessing new and existing products over their entire life cycle has led to the increased use of *life cycle assessments* (LCAs) to document their environmental impacts and even improve product design, manufacture, and disposal. This is partly in response to environmental issues which are increasing in complexity and regulations that are becoming more stringent and globally relevant. However, the reliability of LCAs and the credibility of their results depend heavily on the sources of data used to conduct these assessments. The *life cycle inventory* (LCI) stage in which materials and energy flows are itemized and audited forms the basis for any proposed LCA study. Unfortunately, accessing site-specific, process-specific, or product-specific data is often difficult. Therefore, most LCA practitioners tend to use available average data such as generic data that can be from mixed sources such as the general literature, articles, expert-estimates or industry data, and empirical formulas. In reality, achieving results that are within an order of magnitude of the supposed true results (or perhaps even several magnitudes) may be sufficient for most broad based LCA analysis. This practice is debated extensively: can LCAs present realistic and acceptable results, especially if used as a decision making tool (Fleischer, 2003 and Weidema, 1998). LCA practitioners consider the improved understanding and even resolution to this issue as a practical and valuable enhancement to the analysis results, and any proactive data measures will add to the current data collection and screening strategies. Furthermore, there is the question about the quality of the data behind the collection strategy of surrogate versus site specific or process specific data.

Incorporating data quality management steps into an LCI may help validate and strengthen the end results from an LCA.

1.1 Problem Statement

Most LCA practitioners and researchers use surrogate or "conceptual" data when conducting the first critical stage, or LCI. Conceptual data, which are derived from literature sources, databases, or existing measured processes or products with similar characteristics, are considered a less troublesome and more convenient approach through which researchers can arrive at conclusions efficiently about a process or product within reasonable amounts of time and effort. Trying to access the actual data for a product or process in question is often fraught with obstacles, such as lack of metering to actually measure a flow, regulatory considerations, proprietary issues, or the general lack of communication between different stakeholders. There is also the predictive scenario in which an industry or party is trying to predict *what will be* the effects from a new product or process: the site-specific data does not even yet exist.

However, if important decisions about products and processes are made on the results of LCAs, then data inconsistencies in LCIs must be resolved if LCAs are to be viewed as reliable tools. A major problem is that LCI data often consists of average values from different origins, as compared to site or process specific data (Fleischer, 2003); hence, this data reliability is questioned because an increase in the degree of uncertainty may occur which can affect the confidence in the eventual LCA results.

In addition, several groups call for the inclusion of *data quality measures* in the LCA methodology in order to assess "how good" assumed or outside data might be for LCA purposes. Few approaches are available but there is no widespread agreement on the practicality and usefulness of these approaches on the different types of LCA studies. There does appear to be some preference for using the *pedigree matrix* suggested by Weidema & Wesnaes (1996), coupled with several modifications (NREL report, 2003).

1.2 Scope of Thesis Research

To examine the effects of using surrogate data, a life cycle inventory will be performed on the body surface *pretreatment* process of automobiles; this is the first stage in the painting of vehicles. The thesis will focus on the *zinc phosphating stage* within pretreatment in which the vehicle body-in-white (BIW) is converted to a phosphated coated body. Of the entire pretreatment process, this is the substage that is the most resource intensive. For this pretreatment process, two sets of data will be used: 1) site-specific data; and 2) conceptual data (i.e., surrogate data, literature sources, etc.). It should be noted that all chemical names have been altered and that process and/or facility descriptions modified for reasons of confidentiality.

A unique opportunity exists because this thesis is able to develop a conceptual LCI *as if no site-specific data existed*, and then to develop a site-specific LCI *to compare how "accurate" is the conceptual LCI.* The original LCI categories for the zinc phosphate process investigated include:

1. Material inputs;
2. Emissions and waste; and

3. Energy consumption.

Energy was later excluded from this analysis as only calculated data was provided from one source (i.e., the site specific source), and it is based on electrical drawings of the facility. Obtaining a conceptual source of energy data proved infeasible because the technology varied significantly and no information was ultimately accessible.

Selected inputs from the whole pretreatment process and the zinc phosphating stage are examined. As for emissions, only selected emissions and waste amounts that are specific to zinc phosphate stage alone and not combined or generated from other pretreatment stages will be analyzed and compared. This selection was made since proportioning the amount of waste from this stage versus other pretreatment stages was not possible. This was confirmed through process experts and academic professionals who concurred that there is no practical method to assume or obtain how much of this output waste stream is specifically assigned or apportioned to any particular form of waste (i.e., only the total waste of the complete process is known, but not the proportion of liquid to solid waste relevant to certain stages).

The research will also investigate other issues that may result in different or conflicting values in the details of an LCI, such as looking at existing variations among the chemical constituents and the concentrations of specific products. In addition, meta-data investigation using data quality indicators will be carried on the two types of data to find its usefulness as a data quality management technique.

1.3 Thesis Goals and Objectives

This LCI analysis research will undertake the following:

1. It will perform a life cycle inventory analysis using conceptual and site-specific data to determine the effect of conceptual data on the LCI outcome and how this affects its reliability as decision-making tool.
2. It will examine the usefulness of the pedigree matrix model using a simplified explanation on data quality indicators and assigning respective scores from a previously defined rating system using the site-specific and conceptual data under consideration. If proven useful, it may provide the insight to speed the process needed to include these measures in LCA frameworks set out by organizations, such as the Society for Environmental Toxicology (SETAC) and the International Organization for Standardization (ISO), and to highlight data limitations prior to using them in any study.

1.4 The Functional Unit

The defined functional unit, or normalized unit basis for comparison, is critical to any LCA. Two functional units will be used for describing the parameters in the pretreatment process: a unit mass per vehicle, as well as a unit mass per square meter of the metal substrate (i.e., surface to be painted). This is will be the case for all environmental indicators under consideration, such as resource use, and solid waste or wastewater generated.

Table 1: Examples of suggested indicators and their associated functional unit

Impact category	***Indicator***	***Description***	***Unit***
Resource use	Material consumption	Reported chemical products	g/vehicle or g/m^2
Waste generated	Wastewater (WW) and sludge (solid waste) amount	Canada, Ontario and United States, Ohio reportable waste documents including the wastewater collected from the zinc phosphate stage mainly and the hazardous residue disposed to environment as reported in compounds form.	g/vehicle or g/m^2

Chapter 2: Background to Life Cycle Assessment and the Automotive Painting Process

The relevance of LCA as a recognized environmental management tool that aids both corporate and public decision has received greater attention and methodological development since the beginning of the 1990s. Examples of this include incorporating LCA within the ISO 14000 Environmental Management System (EMS), the European Union (EU) Eco-Management and Audit Scheme (EMAS), and the European Community (EC) Directive on Integrated Pollution Prevention and Control (IPPC), which require companies to have a full knowledge and the environmental consequences of their actions, both on and off-site. A number of corporations and organizations have adopted the method to help them understand the environmental impacts of their actions.

Ideally, the assessment must include the entire life cycle of the product or activity, encompassing extracting and processing raw materials; manufacturing; distribution; use; re-use; maintenance; recycling and final disposal; and all transportation involved (SETAC, 1993). The three stages included in any life cycle assessment are the inventory analysis stage, the impact analysis stage and improvement analysis stage as the following figure shows.

2.1 Life Cycle Inventory

As can be seen from Figure 1, the inventory analysis stage forms the basis for any LCA study and is the basis for evaluating environmental impacts or potential improvements from products, or processes, or services (EPA, 2003). In the current practice, two sources of inventory are typically used to perform LCA studies: conceptual/generic and actual/site-specific data.

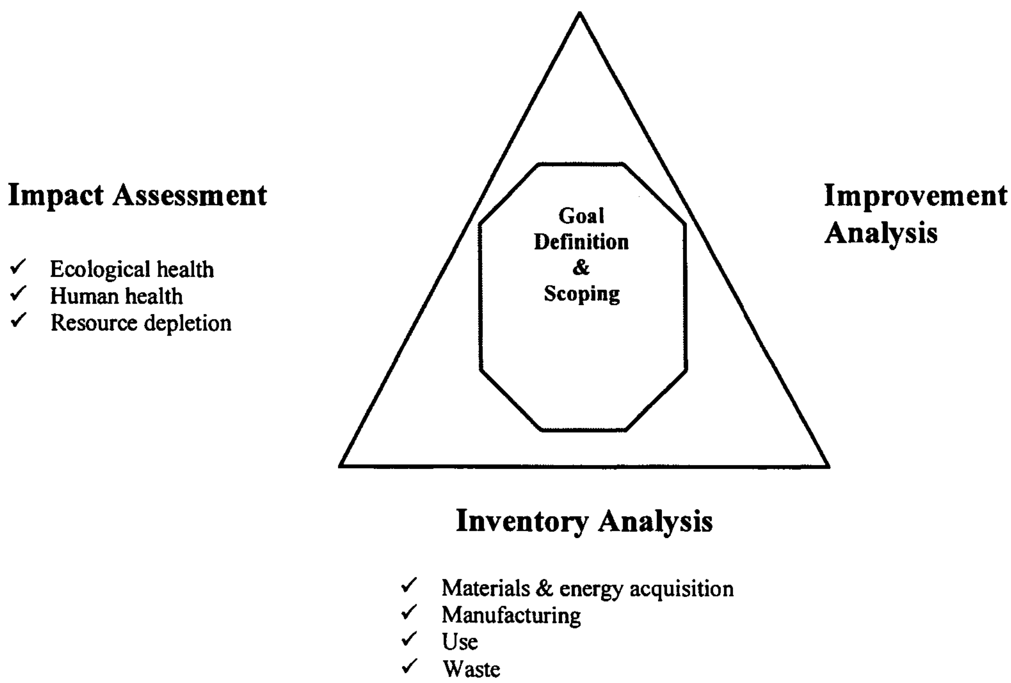


Figure 1: the SETAC depiction of the Life Cycle Assessment (adapted from Hundal)

Although some industries may have inventory databases, accessing them is not an easy task. Several literature sources mention that when trying to compare products using LCA with generic data or less available data, the LCA may have arbitrary cut-off limits in terms of data acquisition because less specific information is known and assumptions had to have been made. As a result, the less documented process may appear more favourable because there is less data available for analysis: fewer resources or lesser emissions may be documented and reported. The end result of such practice raises questions about the reliability in LCA conclusions and outcomes (SETAC, 1998).

2.2 The Automotive Painting Process

Painting serves as a protective, decorative coating that is applied on the vehicle's exterior metallic part that is called the *body in white* (BIW). The prime automotive coatings are used mainly for their anti-corrosive and stone chip resistance characteristics. They also enhance the vehicle aesthetic by providing final durable and appealing finish. This thesis will analyze the inventory data of the most intensive industrial stage within the pretreatment process, which is the first stage in the automotive painting system.

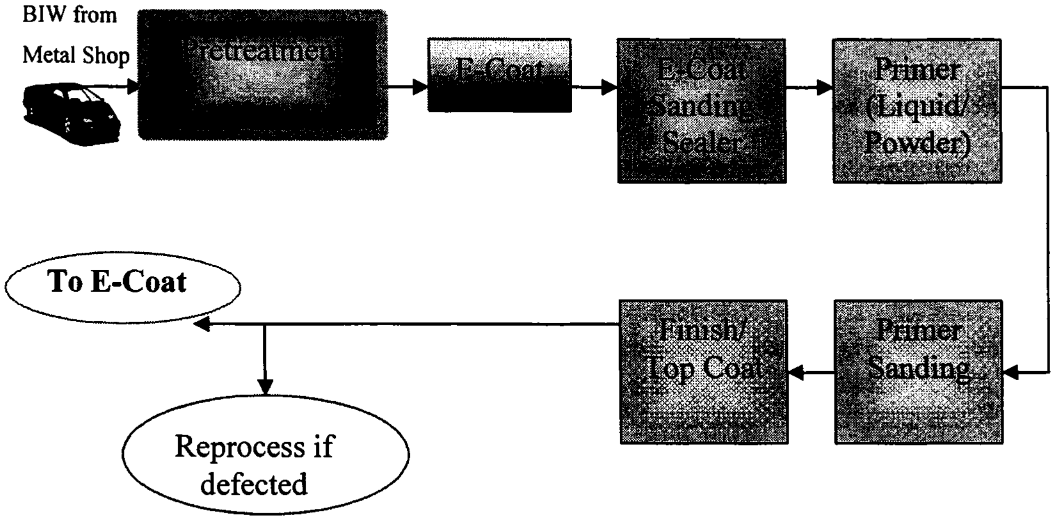


Figure 2: Generalized flow diagram of a typical paint system (after Tighe, 2003)

2.2.1 The Pretreatment Process

Vehicle pretreatment is the first process after the BIW leaves the body shop. The terms phosphating process, phosphate coating, or zinc phosphating process and the pretreatment process are interchangeable, although within this thesis zinc phosphate refers strictly to that substage within pretreatment. However, this substage is the most resource intensive and thus is often used to refer to the entire pretreatment process. At the end of this process a complete zinc phosphate coating is attained on the vehicle's body which provides an inert, protective layer. Pretreating a vehicle's body surfaces has three purposes (Paul, 1996):

1. Removing the mill and pressing oils, and providing a temporary rust protective coating.

2. Securing an inert surface of metal phosphate to enhance paint adhesion for the subsequent primer layer.
3. Providing an anti-corrosive barrier under the paint film. A simplified flowchart of the pretreatment process is shown in Figure 3.

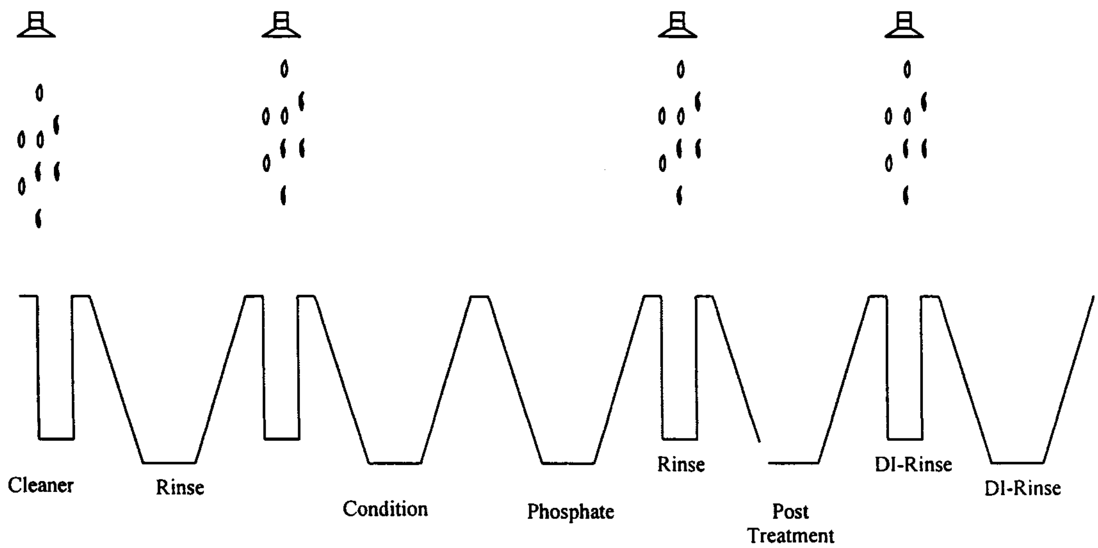


Figure 3: Simplified flowchart of the pretreatment process (after Tighe, 2003)

The pretreatment process is applied in almost all automotive painting facilities. The process usually consists of several steps: cleaning, rinsing, activating, phosphating, sealing or post-rinsing. Some of these operations may be omitted or combined, depending on the application (Weng, 1998). For example, the representative plant in this study uses some aluminium in the vehicle body. As a consequence, the pretreatment process studied may have some additional or different chemicals to allow for this material difference as compared to a "standard" pretreatment process.

2.3 Data Quality Indicators

Indicators describe various aspects of the operation of a program, service, or institution and are typically expressed as an index or ratio. They must be relevant, reliable, and clear (SCOEA, 2003). Indicators that provide information about the properties of the data itself (meta-data) are called *data quality indicators* (DQI). These indicators can improve the confidence in the results of LCI/LCA. Examples of DQI and the issues they represent include:

- Geographical extent or horizon
- Time extent or horizon
- Data precision
- Data completeness
- Data representativeness
- Data source
- Contact person
- Flow chart of the process
- Scope
- Type of scenario handled or needed to be modeled (Weidema and Wesnaes, 1996).

Several of the above mentioned indicators will be examined in relation to the different types of LCI data used in this research. These include the ones identified in the pedigree matrix presented by Weidema and Wesnaes, (1996) such as the reliability and completeness, as well as geographical, temporal, and technological considerations.

2.4 Common Data Sources

MSDS and CAS references are several sources of data which are usually publicly available and can be referred to when developing a conceptual LCI and if site-specific data is not accessible or available.

2.4.1 Material Safety Data Sheets (MSDS)

Material Safety Data Sheets (MSDS) include information about the material in question and focus on the composition for the primary purpose of safety. It includes the chemical's identification and use, physical properties, fire and explosion data, reactivity data, toxicological properties or health hazard data, and preventive measure for spill or leak incidents of the chemical(s). It may also include sections on special protection, special precautions and waste labelling information if needed (Household Products Database, 2004).

2.4.2 Chemical Abstract Service (CAS)

CAS registry numbers also referred to as CAS numbers or CAS RNs are unique numerical identifiers that are considered a valuable collection of substance database especially to recognize and check if different given names of chemicals actually refers to the same substance. This is important from a safety and inventory perspective for chemical compounds. The Chemical Abstract Service, a division of the American Chemical Society, assigns these identifiers. About 20 million compounds have received a CAS number so far, with about 4,000 new ones being added each day. As with MSDS information, CAS information is another form of publicly available information that can be used in an LCI to confirm the consistuents of any compound (Fact-index, 2004; CAS, 2004; ILPI, 2004).

Chapter 3: Project Development and Issues

This chapter discusses the development of this thesis as part of a larger industry initiative, as well as specific issues behind the use of LCIs.

3.1 Automotive LCI Database Background

In early 1990s, the Society of Environmental Toxicology and Chemistry (SETAC) initiated activities to define the LCA technique. *Life cycle assessment (LCA)* is a recognized tool to evaluate the environmental impacts related to technology and industry practices. Following this initiative, the International Organization for Standardization (ISO) developed principles and guidelines on the LCA methodology.

In January 1992, the United States Council for Automotive Research (USCAR) organization was formed by DaimlerChrysler (then Chrysler), Ford and General Motors corporations to find better technological applications of the domestic auto industry through a collaborative, pre-competitive research. Their goals extended to finding new opportunities and sharing joint research outcomes (USCAR, 2003).

One of the initiatives is the Vehicle Recycling Partnership (VRP), a subgroup of USCAR, which has assumed the leadership role among the three large domestic North American automobile manufacturers to compile a life cycle inventory (LCI) database of the various automobile production processes. This thesis is based in part on the research work needed to evaluate the automotive pretreatment painting process for this LCI automotive database.

Results of the complete LCI report will be 'rolled up' or aggregated in order to provide generically applicable data on the life cycle of the automobile and will not be specific to any one vehicle type or manufacturer.

The application and use of the LCI database developed for the USCAR project will be diverse, as interested parties and LCA practitioners will have various objectives or goals. For example, the LCI values of the pretreatment process may be used to assess the process's overall contribution to vehicle impacts. Such a database system should be highly representative of actual processes and of the highest quality possible. It is also ideal to have *documentation* about the data such as time, geographical, and technological correlations (NREL report, 2003), the type of the data used (i.e., conceptual or site-specific) and type of scenario modeled (e.g., normal, best, or worst case scenario) (Weidema and Wesnaes, 1996). Such additional information will allow for the data to be modified and updated.

In general, site and/or process specific data is often not available for parties outside of the industry or corporations. The reasons are many, including confidentiality, proprietary rights, competitive advantage, information misuse or misrepresentation, and possible liability. As a result, "generic" or surrogate data is often substituted. The effects of the data source on LCA results are debated extensively: studies often use a mix of unidentified data sources, assumptions, generalized data, literature sources, and available industry data arising from similar (or perhaps dissimilar) conditions.

3.2 Life Cycle Inventory Issues

LCI studies can be straightforward inventories of the materials and energy flows of a single system, or can compare two or more systems on the basis of providing equivalent function. The results provide an environmental profile of the system(s) studied, such as the main contributors to environmental burdens such as energy use, solid waste, and atmospheric and waterborne emissions, enabling the company, industry, or other stakeholders to effectively target efforts for environmental improvement (Franklin, 2004).

3.2.1 Probable Causes of the Problem in Literature

The diversity of the data sources within the inventory stage result in data quality issues that affect the LCA application as a tool in terms of value, certainty, reliability of the study results, along with the interpretation of the study outcome (Krozer, 1998; Fleisher, 2003; Fava et al. 1994; Weidema and Wesnaes, 1996). The lack of data and lack of representative data can lead to unreliable results (Huijbregts et al, 2001). Surprisingly, this issue was rarely analyzed in previous literature due to the lack of feasible methods and also due to the lack of sufficient reliable data for performing such an analysis (Maurice et al., 2000; Coulon 1997). Lately, there has been a preference for using a quantitative assessment of the uncertainty between a measured 'given' value and the unknown true value. However, this is still considered difficult to achieve and needs further clarification (Huijbregts et al, 2001). There are several controversies related to the use of quantitative assessment among the people who perform LCA. On one hand most researchers find that there is a need to apply uncertainty analyses in order to understand the LCA results (Krozer, 1998; Fleisher, 2003; Fava et al. 1994; Weidema and Wesnaes, 1996). On the other hand, others who have used these analyses advocate that uncertainty is currently not a significant issue (Ross, 2002).

This assertion contradicts earlier conclusions that uncertainty is an important issue affecting LCA results (Huijbregts et al, 2001; Maurice et al., 2000; Weidema and Wesnaes, 1996). Fleischer (2003) refutes most of the early calls to include data quality management unless uncertainty factors are introduced to assess the correlation quantitatively between used and needed data. As a result concerns about the outcome of LCAs studies due to low quality data will be reduced (Weidema and Wesnaes, 1996).

The effect of the LCI data type is an important topic. LCA users need additional clarification about its reliability, especially with the increased use of LCA in corporations to identify areas where improvements can be made, and sometimes to market and claim the environmental superiority of their products (GDRC, 2003).

3.2.2 Limitations of Using Conceptual or Surrogate Data

For processes data sets, the inclusion of auxiliary processes that are based on average conditions is typical. As a result, this situation is ranked as "poorly documented" and when combined with a high level of data aggregation, can lead to errors. Sources of errors can include double-counting. Also, a disadvantage of using generic data appears to be the transfer of generic data to a specific application. This leads to a downgrading in the accuracy of the results because additional systematic errors may be incurred (Fleisher, 2003). In addition, the quality of the input data is a limiting aspect in LCA results (Coulon, 1997). As a result, it is not advisable to disregard data quality management tools such as uncertainty analysis and the pedigree matrix (Weidema and Wesnaes, 1996) because they can improve the creditability of LCAs (Maurice et. al, 2000). Some additional development of LCA in the areas of data quality management such as Data Quality Indicators (DQI) along with industrial process modeling should be helpful in promoting its usefulness (Sullivan, 1998). Nevertheless, the research into easier methods for applying data quality management tools is ongoing (Ciroth, 2001). Krinke (2003) compared the effects of including data quality measures on the Global Warming Potential (GWP) impacts using a case study of two automotive front ends and concluded that inclusion of some "poor" quality data can change the GWP results.

3.3 Improving Life Cycle Inventory Analysis

Because using generic data is recognized as a common practice in LCA studies and its effect of the LCA conclusions are debated among the LCA community, a few efforts attempted to make generic data more applicable, such as checking the appropriateness of the data in the context of the respective goal and scope of the study. For example, (Fleischer, 2003) attempted in one approach to apply generic data for a transportation process to a specific situation by factoring in the transportation distance. The same researcher attempted in a second approach to use average data to fill data gaps in small and medium enterprises processes. It was assumed that the resulting changes in these smaller systems would be modest (Fleischer, 2003). However, systematic errors in LCAs conducted even in smaller scale industries can still exist (Fleischer, 2003). Presumably, accessing site-specific data would make a difference in LCA results, or at least, determining the approximate differences between generic data and situation specific data.

Others (Coulon et al. 1997) called for including uncertainty analysis to improve decision making. They advised that including the source of actual data is the best provider of information for describing the type and statistical distribution of data (if applicable) but only if the study goal and objectives are clearly defined. They found if actual data is lacking then expert judgment can be implemented to quantify the distribution of the input data; however, much depends on the ability of the expert.

In addition (Coulen et al. 1997) argue that not all LCI data categories present the same uncertainty. For example, in Table 2, when three different sites of plastic manufacturers were compared using actual and expert judgment data, each situation resulted in significantly different values for inventory categories. Though Coulon et al. (1997) criticize aspects of the DQI and stochastic models, they concluded that mixed approaches of these methods and an estimate on confidence level should be implemented in future studies of LCAs. This is especially true because of the increasing awareness of the public of the underlying uncertainty and complexity of the final results from LCA studies.

Table 2: Range of the various inventory data categories taken for three-polymer production processes (adapted from Coulon et al., 1997)

	Min.	Average	Max.
Energy	0.86	1.0	1.3
Main air emission	0.18	1.0	2.9
Water effluents	0.01	1.0	17.0
Hazardous solid waste	0.00	1.0	21.0
Non-hazardous solid waste	0.05	1.0	2.8

Furthermore, previous literature references (Weng, 1998) are criticized because they performed an LCA study to evaluate impacts of the pretreatment process without mentioning how inventories were obtained. The assembly line that was studied treats about 1500 square meter per hour, which is about one fourth of a modern facility's ability (Lambourne et al, 1999), yet this article gives the impression that vehicle pretreatment processes should have more or less similar impact values. The effects of different physical scales, the passage of time and therefore technological advancement, and different geographical locations are not well known.

3.4 Using Conceptual or Surrogate Data

Studies that investigated the use of generic data in LCA studies (Fleischer et al, 2003) made no clear recommendation in this regard. In addition the authors used data that could come from unrelated industries, "average" values, and so on. In this proposed research, the conceptual data used is derived from relevant facility processes and data from paint process theories, automotive LCA databases, similar paint facility data (surrogate data) or the expertise from paint experts. Such data is likely to be more applicable than generic data.

3.5.1 Definitions of terms used in this research

Generic data is data that can be considered generally applicable ("typical data") but is not necessarily specific to the industry or process being studied. It can come from a variety of literature sources and databases. For example, when determining the impacts of transporting goods, typical truck fuel efficiency values may be used irrespective of the actual mass or type of goods being moved, the geographical locations traveled through, or the blend of fuel consumed.

Surrogate data is data that comes from an actual facility or process that appears to be similar to the one being studied and thus may be accepted at "face value". However, in this research, surrogate data assumes that there is little or no opportunity to confirm the degree of applicability of such data to the site specific facility or process. The LCI practitioner may have to assume that surrogate data - by virtue of coming from the same type of facility or process – is superior to generic data.

Conceptual data refers to the combination of surrogate data supplemented with generic data to fill in data gaps.

Site-specific data is on-site, process-specific data derived from actual measurement records, expert judgment, or circumstance specific calculations.

Product refers to the input amount of a specific material or item used in the pretreatment process stages, such as a chemical cleaner or replenisher.

Constituent refers to the individual chemicals that make up a product and can be listed as inputs or outputs to or from a system or process stage (e.g., phosphoric acid, nickel nitrate).

Chapter 4: Data Sources and Data Quality Assessment

The *site specific data* in this research was derived from the pretreatment paint process at "Facility A". The *conceptual data* consisted of surrogate data derived from the pretreatment paint process data at "Facility B" and was supplemented by generic data from literature sources, online databases, supplier or industry wide MSDS, etc. Both facilities are located in North America but in different jurisdictions. This comparison is ideal in that it represents a situation faced by LCA practitioners: data from one facility under similar but not exactly the same regulatory requirements will be used to model a facility in a different regulatory environment.

A key aspect of this research was to critically analyze several sources of MSDS documentation that provide information about the products' constituents and concentrations. Realistically, this source of data can be very useful to the LCA practitioner, especially if faced with many data gaps. MSDS documents from several sources were obtained and will be explained in the next chapter.

4.1 Description of the Two Plants under Consideration

Two main sources of the process-specific data that were analyzed include:

1. Facility A's production of current generation vehicles began in 2000. At full capacity, the plant implements a three shift schedule and is able to produce about 1325 vehicles per day, or about 335000 vehicles annually. Facility A produces two vehicles from two different platforms. Although it is an older facility,

Facility A's pretreatment process has been retrofitted to current practices and standards.

2. Facility B is a newer plant than Facility A and produces vehicles using a lean manufacturing model. At full production, vehicle production is estimated to be 800 to 966 vehicles per day, or 249,000 units annually on a two-shift operation. This facility represents the culmination of best practices from the company's worldwide manufacturing operations for lean, flexible, high-quality production and represents state-of-the-art manufacturing processes.

4.2 Data Quality

To examine data quality, the *pedigree matrix* by (Weidema and Wesnaes, 1996) will be used. This matrix consists of five data quality indicators that are described as adequate and sufficient parameters for evaluating data quality issues relevant to the LCI data. Table 3 shows the different indicators and the authors' evaluation score or rating system.

Table 3: Pedigree matrix with 5 DQI (adapted from Weidema and Wesnaes, 1996).

Indicator Score	***1***	***2***	***3***	***4***	***5***
Reliability	Verified data based on measurements	Verified data partly based on assumptions or non-verified data based on measurements	Non-verified data partly based on assumptions	Qualified estimate (e.g. by industrial expert)	Non-qualified estimate
Completeness	Representative data from a sufficient sample of sites over an adequate period to even out normal fluctuations	Representative data from a smaller number of sites but for adequate periods	Representative data from an adequate number of sites but for shorter periods	Representative data but from a smaller number of sites and shorter periods or incomplete data from an adequate number of sites and periods	Representativeness unknown or incomplete data from a smaller number of sites and/or from shorter periods
Temporal correlation	Less than three years of difference to year of study	Less than six years of difference	Less than 10 years difference	Less than 15 years difference	Age of data unknown or more than 15 years of difference
Geographical correlation	Data from area under study	Average data from larger area in which the area under study is included	Data from area with similar production conditions	Data from area with slightly similar production conditions	Data from unknown area or area with very different production condition
Further technological correlation	Data from enterprises, processes and materials under study	Data from processes and materials under study but from different enterprises	Data from processes and materials under study but from different technology	Data on related processes or materials but some technology	Data on related processes or materials but different technology

The two main purposes for applying such a matrix in this study are:

1. To find the practicality and efficiency of literature proposed methods in identifying the strengths or weaknesses within LCI data;
2. To investigate the usefulness of including such procedures as a part of any future LCA. Many LCA practitioners are very concerned with data quality in LCA studies (NREL report, 2003).
3. Each DQI will score a value between 1 and 5 where 1 refers to the "best" rating and 5 is the "worst", as shown in Table 3. After that the scores will be compiled in the proposed format (e.g., 2, 3, 1, 2, 5) that highlight weaknesses in the data. This is explained further in Chapter 5.

Chapter 5: Research Analysis

A comparable analysis of the two data sets will be carried out to test how close an LCI derived from surrogate or conceptual data approaches to one using site-specific information.

5.1 Data Collection

The site specific data from Facility A consisted of internal reports, government reported amounts, and on-site expert estimates. Outside sources (e.g., MSDS) were also used out of necessity, but every effort was made to find site specific MSDS documents.

Examples of the surrogate data available from Facility B included the total amounts of products used on an annual basis in the zinc phosphate stage. These were specified in government documents that report these annual usage amounts. Each product was broken down into a group of chemical compounds. Along with the name of these chemicals their average percentage or concentration was also provided the amount used was calculated by averaging the high and low concentrations of the compounds and multiplying this percent by the total quantity of the product used.

The surrogate data also presented data found in the U.S. Toxic Release Inventory reports (TRI). TRI emission data combine amounts of compounds from several pretreatment stages and report it as one amount. This amount is proportioned into several streams such as the amounts emitted to air, amount adhered to metal, or consumed in process

(CIP). The remaining waste is treated in a wastewater treatment plant and sent to landfills as sludge or discharged as wastewater. As a result, setting the boundary limits around any separate stage in the pretreatment process was difficult because it was usually not clear or obvious how amounts and flows could be divided among individual stages. Significant assumptions were needed to simplify the scenario and focus on the emissions used in the zinc phosphate stage. Combining the surrogate data with data from available literature and industry databases forms the *conceptual data* that will be used to approximate an LCI for a process.

5.2 Collection of Product Information Documents

The thesis work required using MSDS from several sources to either supplement or complement the conceptual data, and to confirm the site-specific data. However, it was discovered that MSDS documents are not necessarily consistent: even if under one manufacturer and one supplier and for the same product, the MSDS documents could vary significantly, depending on the provider of the actual MSDS. Each of the MSDS sources used in this research is described briefly below.

1. The documents that were provided from the surrogate data source are not strictly MSDS, but can be considered equivalent to MSDS for this research. The documents included the product name, its constituents and their respective concentration (a mean value of the given higher and lower concentration was provided on these documents) for selected main chemicals. The less significant chemicals were excluded as well as the water types such as city water, or deionized water percentages. They represent information from the year 2001 and will be termed *Facility B TRI*.

2. A second source of MSDS - *online source* - comes from mostly online references that are increasingly available and potentially useful if LCA practitioners lack time or the ability to acquire site specific data. This type of data can also be valuable for filling in data gaps.
3. A third source is MSDS directly supplied from the supplier for the products used in the pretreatment process. It is usually the most recent version available and it contains more detailed information on all constituents involved in any product's formula. This type is identified by the name *Detailed MSDS.*
4. A fourth source of the MSDS was supplied from the automotive manufacturer. These are not specific to any facility but to all similar processes within the corporation. This is termed *Corporate MSDS.* Their format was not easily readable and was likely intended for internal company use only.
5. A fifth source of MSDS was specific to Facility A and was found to differ from the broader corporate MSDS and the supplier's MSDS. These have fewer details than the paint suppliers' MSDS but serve as an additional useful source of comparison. In addition, Facility A National Pollutant Release Inventory (NPRI) documents can be used as an additional source of MSDS-type data because they provides actual consumption amounts and concentrations of compounds as reported to the government. All MSDSs sources that are made available regarding this process are used for comparison purposes.

5.3 Thesis Research Specifics

The difference between conceptual and site-specific LCI values will be calculated using two functional units, g/vehicle and g/m^2. This will also demonstrate the effect of using various functional units on the analysis results.

The surface area of a body-in-white that is exposed to pretreatment is reported from the site-specific facility for two vehicle platforms: V1 with an area of 146 m^2 and V2 with an area of 151.5 m^2. This measured value was provided using detailed CAD information and gives an average area of 148 m^2, which will be used throughout this study unless stated otherwise. This area includes all interior and exterior metal surfaces, including door panels. A hand measured estimate of this same vehicle's surface area to be 45 m^2, which is about third of the actual reported pretreated area. This substantial difference suggests why site specific data could be preferred in many situations. However, the average surface area of vehicles in the facility representing surrogate data was not reported. Therefore, an alternative value was found in Table 4.2.2.8-2 of the *Light Duty Truck Surface Coating* (EPA, 2004). The table listed range of the area of prime coating to range from (850-1250) ft^2 this was averaged to 1100 ft^2, which is equivalent to79 m^2, 116 m^2 or 102 m^2 respectively. For this analysis, the higher limit of the area (1250 ft^2 or 116 m^2) was used because it more closely matches the vehicle produced at Facility A, and as a result, is closer to the actual reported vehicle area. This difference from the site specific reported 148 m^2 may be due to variations in the size of the vehicle considered in literature or the age of the information in that reference.

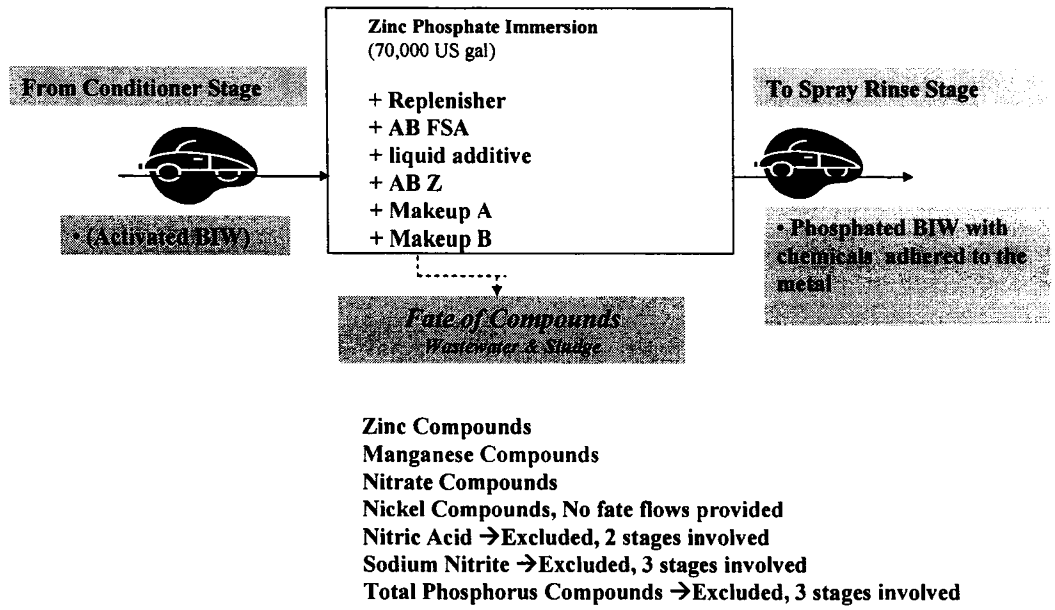
Even determining the number of vehicles produced is not always straightforward. One source at the site specific facility reported 287,127 vehicles produced from January 2003 to December 2003. This differs from the production amount corresponding to the NPRI yearly report that extends from May 2002 to May 2003. However, this value is considered a close estimate and will be used whenever NPRI values are implemented in the analysis; it would have been preferable if this value could be confirmed with other on-site production values. Another value that was reported from Facility A and checked was the production figures from August 2003 to May 2004 which corresponds to 245,472 vehicles in ten months. This value represents the supplier's on-site records that listed the products and materials consumed in the pretreatment stage along with the vehicles produced during that period. When extrapolated to a full calendar year, this ten month production value is reasonably close to the overall 287,127 reported previously. For the conceptual data, the annual vehicle production rate is estimated from several literature and conceptual sources to be well over 200,000 units annually but less than the plant's full capacity, or 249,000 vehicles annually: an average value of 224500 vheicle is used as there was no measured vehicle production data from the Facility B available to the researschers.

Emissions wise, it was only possible to carry out a comparable LCI analysis of certain waste amounts that were reported from both facilities using Facility A NPRI 2003 data versus Facility B TRI 2001 data. These mainly apply to compounds in the zinc phosphate stage that include hazardous heavy metals compounds including zinc, manganese and nickel compounds.

In applying the pedigree matrix it is expected that the life cycle inventories from both the plants will score "1" reflecting the "best" data quality scenario with respect to the temporal correlation: both facilities is generally less than three years. For the geographical correlation, Facility A scores a "1" because all the data comes from the area under study, while Facility B data comes from a larger area and so will score "2". For the technological correlation, the data from the conceptual facility represents the same pretreatment process but comes from a different facility with different technologies in place. As a result, Facility A scores 1 in this aspect while Facility B scores 2.

Chapter 6: Research Analysis & Discussion

The comparative LCI analysis is performed on the zinc phosphating stage illustrated in Figure 4 below. The analysis will also include selected aspects of the entire pretreatment process to provide additional insights into LCI data issues.



* Products could still be present from previous/current stages are considered negligible trace amounts
Note: Makeup A & B are used as needed.

Figure 4: The zinc phosphate stage in the pretreatment process representing Facility "A"

The phosphate stage shown in Figure 4 follows the conditioner stage where the body is activated to receive the zinc phosphating coating. The chemistry of this process begins as the phosphate crystals grow from solution onto the metal surface until the coating completely impregnates the metal and covers the whole surface. This crystalline structure results from the metal phosphates of different chemical forms and the equilibrium that exists in the aqueous acid solution.

6.1 Comparison of Selected Products Used in Pretreatment Using Conceptual versus Site Specific Data

Tables 4 through 7 and the accompanying figures compare selected LCI inputs reported for the whole pretreatment process from Facility A and Facility B and the differences between the conceptual and site specific data sources. The specifics of this analysis include:

- Facility A average pretreated surface area for a vehicle is 148 m^2.
- Facility B estimated surface area for a vehicle was taken as the upper limit prime coat area of a light duty truck from literature is 116 m^2. The other surface areas of 79, 102 and 116 m^2, which are also available to a LCI practitioner, will be used in addition to the hand measured estimate of 45 m^2 in a sensitivity analysis.
- Facility A site specific production rate corresponding to the period August 2003 to May 2004 is 245472 vehicles and is used in Table 4 (measured for ten months period by a facility expert). 287127 vehicles reported for the calendar year January to December 2003 by a non-facility expert is used in table 5.
- Facility B estimated production rate corresponding to the 2001 reporting year using literature/online sources is an average 224500 vehicles.
- Facility B data source reflects the 2001 reporting year Toxic Release Inventory (TRI).
- Facility A data comes from site-specific records, as well as the 2003 reporting year for the NPRI

Table 4: Comparable analysis of products used in the pretreatment process using conceptual TRI documents vs. site-specific usage records in g/vehicle

S/No.	*Product Name*	Stage	Product Usage Amount in (Lbs)		Amount in (Lbs/vehicle)		Usage Amount in (g/vehicle)		Difference = Site-Specific-Conceptual (g/veh)	% Difference g/veh
			Conceptual TRI reports	Site-Specific Records	Conceptual TRI reports	Site-specific Records	Conceptual TRI reports	Site-Specific Records		
1	*Chemical cleaner*	*Pre-clean*	99186	231368	0.44	0.94	200	428	*227*	**53**
2	*Conditioner*	*4*	40993	47390	0.18	0.19	83	88	*4.7*	**5**
3	*Replenisher*	*5*	577200	847422	2.57	3.45	1166	1566	*399.*	**26**
4	*Liquid Additive*	*5*	60840	91849	0.27	0.37	123	170	*46.8*	**28**
5	*Chemical controller*	*7*	705	91575	0.00	0.37	1.4	169	*167.8*	**99**

Note: Site-specific product usage amounts in Table 4 reflect a ten month period reported using supplier's measured records, while the conceptual source depends on (TRI) data. The corresponding vehicle production to these amounts are 245472 and 224500 vehicles respectively.

Table 5: Comparable analysis of Products used in the pretreatment process using conceptual TRI documents vs. site-specific NPRI documents in g/vehicle

S/No.	Product Name	Stage	Product Usage Amount in (Lbs)		Amount in (Lbs/vehicle)		Usage Amount in (g/vehicle)		Difference = Site-Specific-Conceptual (g/veh)	% Difference g/veh
			Conceptual TRI reports	Site-Specific NPRI Reports	Conceptual TRI reports	Site-specific NPRI Reports	Conceptual TRI reports	Site-Specific NPRI Reports		
1	*Chemical cleaner*	*Pre-clean*	99186	228811	0.44	0.80	200	361	*161.1*	**45**
2	*Conditioner*	*4*	40993	X	0.18		83			
3	*Replenisher*	*5*	577200	868608	2.57	3.03	1166	1372	*205.9*	**15**
4	*Liquid Additive*	*5*	60840	X	0.27		123			
5	*Chemical controller*	*7*	705	103204	0.00	0.36	1.4	163	*161.6*	**99**

Note: The Site-specific usage amounts in Table 5 are taken from NPRI reported data and normalized while the conceptual source depends on (TRI) data. Vehicle production corresponding to the amounts are 287127 and 224500 vehicles respectively.

Table 6: Comparable analysis of Products used in the pretreatment process using conceptual TRI documents vs. site-specific usage records in g/ m^2

S/No.	Product Name	Stage	Product Usage Amount in (Lbs)		Usage Amount in (Lbs/vehicle)		Usage Amount in (g/ m^2)		Difference = Site-Specific-Conceptual (g/m^2)	% Difference (g/ m^2)
			Conceptual TRI reports	Site-Specific Records	Conceptual TRI reports	Site-specific Records	Conceptual TRI reports	Site-Specific NPRI Reports		
1	*Chemical cleaner*	*Pre-clean*	99186	231368	0.44	0.94	1.72	2.89	*1.17*	**40**
2	*Conditioner*	*4*	40993	47390	0.18	0.19	0.71	0.59	*-0.12*	**-17**
3	*Replenisher*	*5*	577200	847422	2.57	3.45	10.05	10.58	*-0.53*	**5**
4	*Liquid Additive*	*5*	60840	91849	0.27	0.37	1.06	1.15	*-0.09*	**9**
5	*Chemical controller*	*7*	705	91575	0.00	0.37	0.01	1.14	*1.13*	**99**

Note: The usage amounts in Table 6 reflect a ten month period reported using site-specific records, while the conceptual source depends on (TRI) data. Vehicle production of 245472 and 224500 vehicles, and surface areas of 148 m^2 and 116 m^2 from Facilities A and B are used respectively.

Table 7: Comparable analysis of Products used in the pretreatment process using conceptual TRI documents vs. site-specific NPRI documents in g/ m^2

S/No.	Product Name	Stage	Product Usage Amount in (Lbs)		Usage Amount in (Lbs/vehicle)		Usage Amount in (g/ m^2)		Difference = Site-Specific-Conceptual (g/m^2)	% Difference (g/ m^2)
			Conceptual TRI reports	Site-Specific NPRI Reports	Conceptual TRI reports	Site-specific NPRI Reports	Conceptual TRI reports	Site-Specific NPRI Reports		
1	*Chemical cleaner*	*Pre-clean*	99186	228811	0.44	0.80	1.72	2.44	*0.48*	**30**
2	*Conditioner*	*4*	40993	X	0.18		0.71			
3	*Replenisher*	*5*	577200	868608	2.57	3.03	10.05	9.27	*-2.16*	**-8**
4	*Liquid Additive*	*5*	60840	X	0.27		1.06			
5	*Chemical controller*	*7*	705	103204	0.00	0.36	0.01	1.10	*1.09*	**99**

Note: The site-specific usage amounts in Table 7 are taken from NPRI data and normalized while the conceptual source depends on (TRI) data. Vehicle production corresponding to 287127 and 224500 vehicles are used for Facilities A and B respectively, and same areas are used as mentioned above.

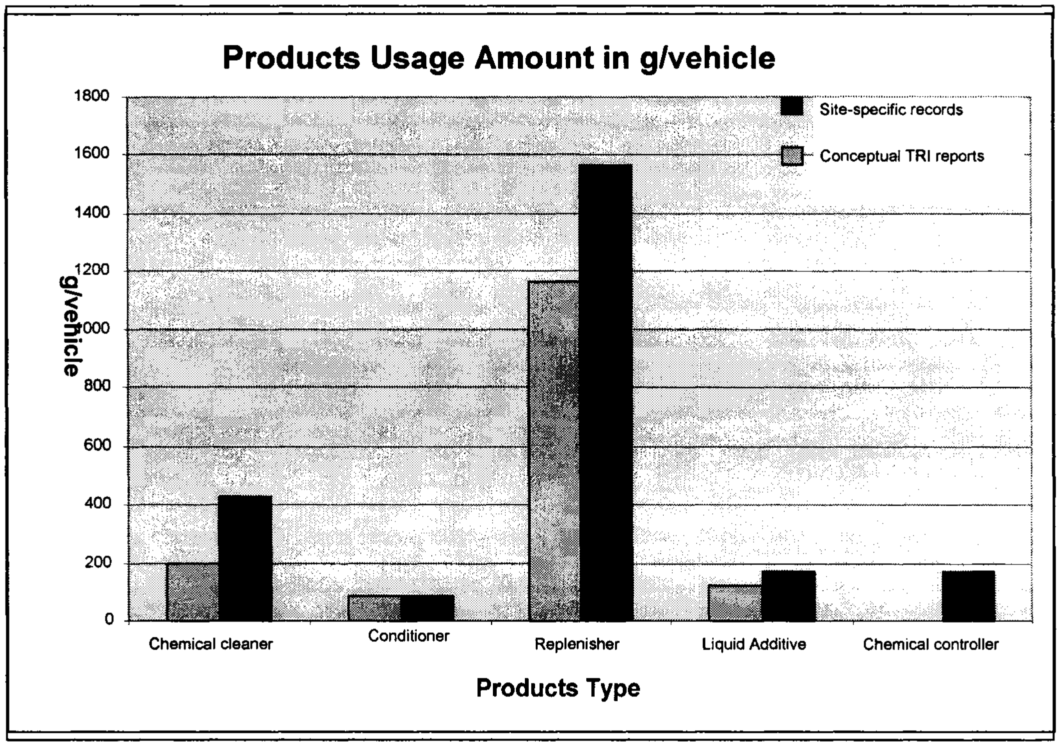


Figure 5: Product usage amount comparison in g/vehicle using site-specific records vs. Conceptual TRI reports as shown in Table 4.

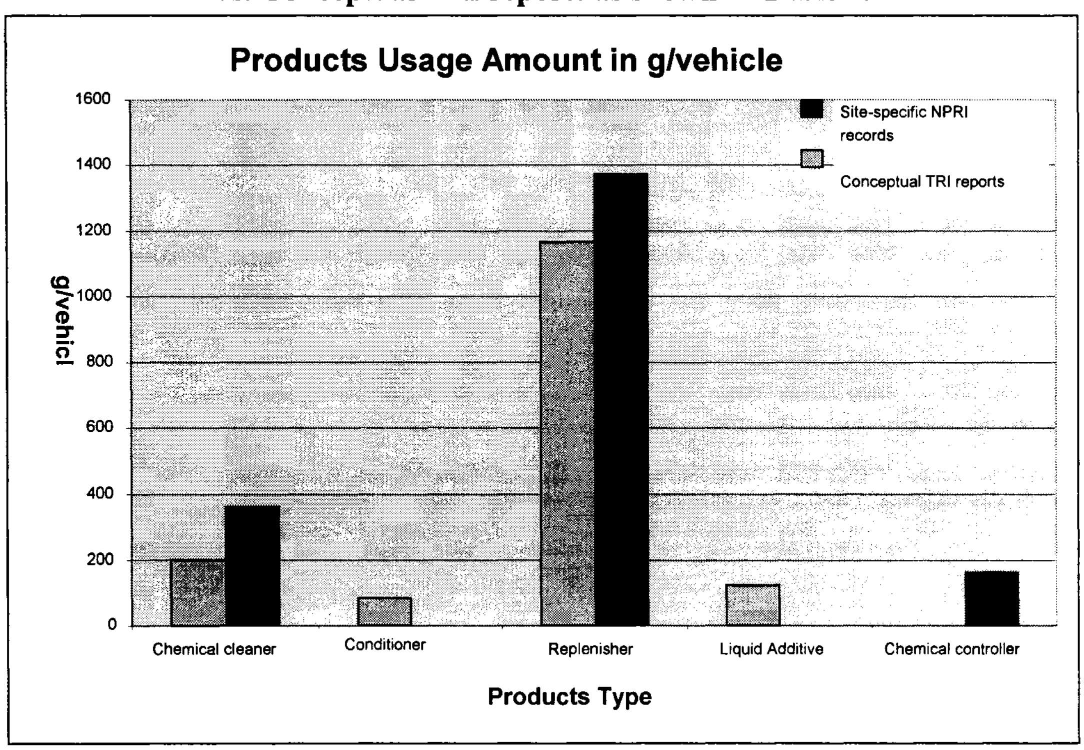


Figure 6: Product usage amount comparison in g/vehicle using site-specific NPRI reports vs. Conceptual TRI reports as shown in Table 5.

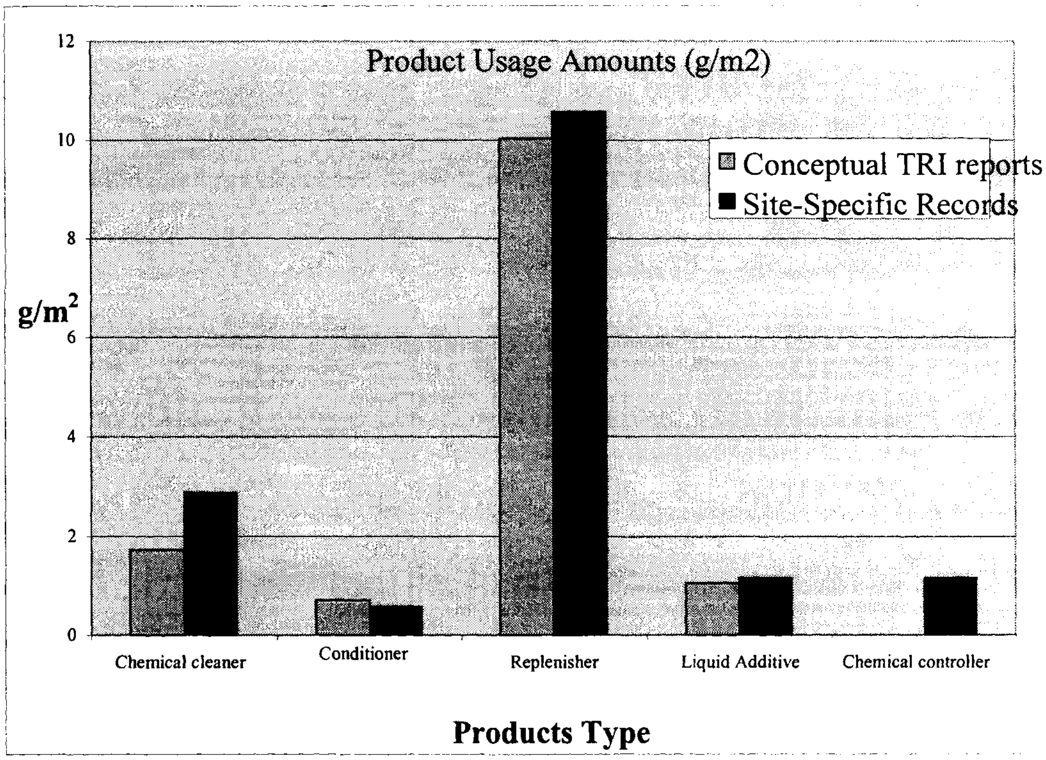


Figure 7: Product usage amount comparison in g/m^2 using site-specific records vs. Conceptual TRI reports as shown in Table 4.

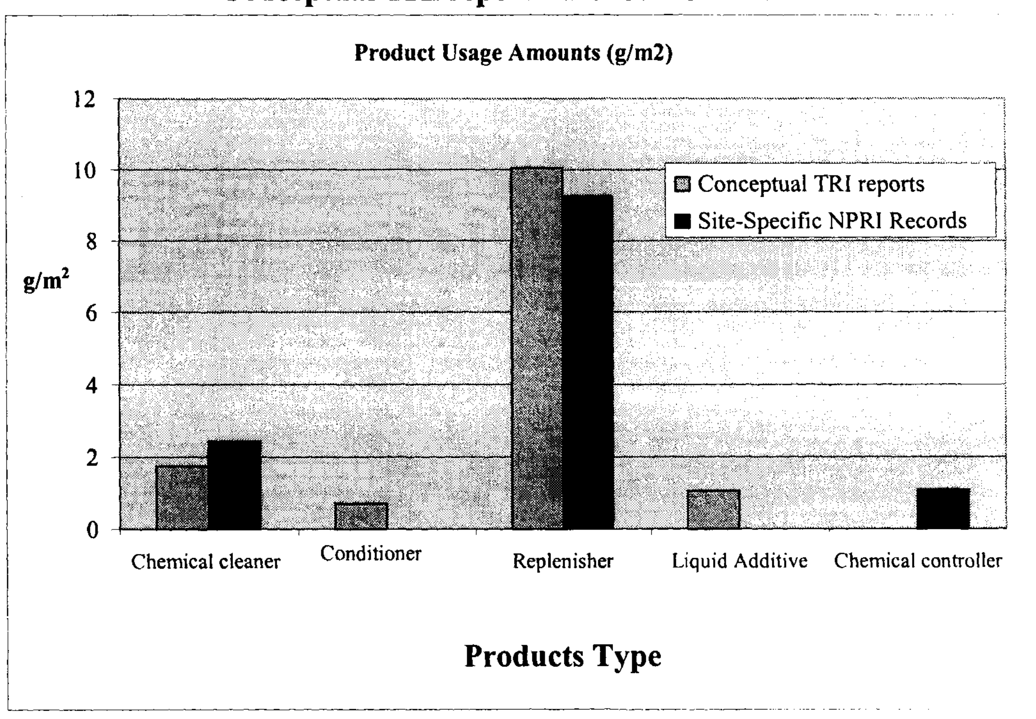


Figure 8: Product usage amount comparison in g/m^2 using site-specific NPRI reports vs. Conceptual TRI reports as shown in Table 5.

6.1.1: Discussion of Pretreatment Data Comparison

The products in the above tables were chosen due to their usage in large quantities within the pretreatment process, because of their contribution to several emissions such as VOC emissions resulted from chemical cleaners, or because of the use of heavy metals (Zn, Mn, Ni) in products such as in the replenisher, possibly resulting in hazardous waste generation. Tables 4 and 5 have the same conceptual source (TRI) data from Facility B. However, the site-specific data from Facility A in Table 4 comes from on-site usage records provided from the process experts. In Table 5, Facility A data comes from the (NPRI) data for the 2003 year. All values are expressed in gram per vehicle unit. The same data arrangement holds for Tables 6 and 7. The above comparisons indicate several shortcomings in using conceptual versus site specific LCI data.

1. In Tables 4 and 5 and Figures 5 and 6, when the g/vehicle unit is used, Facility A seems to use more products in as compared to Facility B in general. Therefore, the percent difference between the conceptual and the site-specific source varies from 5% to 99% in Table 4, or 15% to 99% in Table 5.
2. Similarly, when the g/m^2 unit is applied in Tables 6 and 7 and Figures 7 and 8 the range of percent differences between the two data sets still vary considerably as mentioned in previous point. In addition to that, some product usage amounts that are reported using two sources from the same Facility A show inconsistent behaviour; for example, the replenisher amount at Facility A in Table 6 reported as $10.58 g/m^2$ which is greater than Facility's B amount (i.e. $10.05 g/m^2$), while in Table 7 Facility A reports less usage amount than facility B. This variability in

results can be due to the differences in the normalizing values of surface area and vehicle production and lower total usage amounts.

3. Tables 4 and 5 in g/vehicle units indicate that modern or state-of-the art plants had some of their current applications improved for better environmental practices by using fewer hazardous chemicals. An example from Table 4 is the chemical controller that includes chemicals such as nitric acid, ethanolamine and zirconate among its constituents. Its usage is largely reduced from 1.4g/veh in the conceptual source as compared to 169 g/veh at the site-specific source. Conceptual source data represents less products are used when the g/vehicle unit is used. The amount in g/m^2 could be less if the area assumed for normalization is underestimated. Which values should be used as reference clearly depends on the process specifics and its related technology.
4. The calculated difference amounts between the two data types may be misleading because the difference varies with the functional unit applied. For example, in the tables above the chemical cleaner and conditioner. For the chemical cleaner, when the functional unit g/m^2 unit is used, the difference between conceptual and site-specific data is equal to 1.17 g/m^2. If the g/veh functional unit is used, the difference is equal to 227 g/veh. These result in differences of 40% and 53% respectively. Similarly, the conditioner has differences of 0.12 g/m^2 and 4.72 g/vehicle, or percentage differences corresponding to 17% and 5% respectively. This indicates the difficulty in assigning a universal correction factor or any type of relationship to describe such variations. Reasons for such differences may be due to the lack of verified information about the surface area and number of the vehicles pretreated.

5. Not only do product usage amounts differ, but there are also naming conflicts. For example, the product chemical controller was reported under different names in each facility, but have the same constituents at both the surrogate and site specific facilities. As a result, product names may be mistakenly named by different facilities or groups, or reported differently.

To confirm these observations, and to determine if there is a consistent amount of difference between the analysis resulting from the conceptual and site specific data, selected aspects of the zinc phosphate stage were checked, starting with the products used, their constituents, their concentration, and finally the emissions.

6.2 Comparison of Selected Products in the Zinc Phosphate Stage Using Conceptual and Site Specific Data

Table 8 below shows the variations that may exist in acquiring information about the products used at a process from a site specific data source versus a conceptual data source.

Table 8: Comparing the list of products used in the zinc phosphating stage

	Product/ Chemical Compound	**Product Reported**	
		SITE SPECIFIC	**CONCEPTUAL**
1	*Replenisher*	√	√
2	*AB FSA*	X	
3	*Liquid Additive*	√	√
4	*AB Z*	X	
5	*Makeup A*	√	
6	*Makeup B*	√	√

√ the product and its amount in pounds was provided from the facility.
X on-site expert or the process flow charts verified the use of the product at the facility but its amount is not provided.

6.2.2 Discussion of Zinc Phosphate Comparison

As shown in the table above, six products were listed from the site specific sources as compared to three products from the conceptual source (specifically, the TRI reported appendices for the surrogate facility). This information could later be misleading for evaluating impacts from the LCI because some products may not be reported depending on the regulatory minimum threshold reporting requirements.

The usage amounts of these products reveal that the replenisher, liquid additive, and makeup B quantities were reported from both facilities. As for the makeup A product, it was only reported from the site specific facility's NPRI appendix, while the usage amounts of the remaining products (AB-Z, and AB-FSA) were not reported from any source in any manner. Even with the cooperation of site experts and readily available information databases, there are still data gaps.

6.3 Comparison of product composition in the zinc phosphate stage using conceptual and site-specific data

The products used in stage 5 are selected to show the differences that may be found between the products constituents of the site-specific data sources versus the conceptual data sources.

Table 9: Difference in listing the products' constituents using the two site-specific sources against the conceptual's TRI source

S/No.		*Product/ Chemical Compound*	Comments	CAS. No.	Source of CAS No. & Year of Data Revision		
					Site Specific MSDS Documents	Site Specific NPRI Documents	Conceptual TRI Documents
1)		**Replenisher**			2003	2003	2001
	1	Phosphoric Acid		**7664382**	√	√	√
	2	Zinc Nitrate (Zn(NO3)2		**7779886**	X	X	√
	2	Zinc Oxide	Assumption: ZnO reacts w/NO2 to form Zinc nitrate	**001314-13-2**	√	√	X
	3	Manganese Phosphate Mn(H2PO4)2		**10124546**	X	X	√
	3	Manganese Monoxide		**1344-43-0**	√	√	X
	4	Nickel Nitrate Ni(NO3)2 (Nickel Salt Solution-14% Nickel)		**013138459**	√	√	√
	5	Zinc Dihydrogen Phosphate ($Zn(H_2PO_4)_2$)		**13598373**	X	X	√
	6	Ammonium Fluoride ((NH4)(HF2)		**001341-49-7**	√	√	X
	7	Nitric Acid		**007697-37-2**	√	√	X

2)		**AB FSA**			**2003**	**2003**	**2001**
	1	Potassium Fluoride Solution (40%)		**7789-23-3**	√	X	N/APP
	2	Ammonium Hydrogen Fluoride		**1341-49-7**	√	X	N/APP
3)		**AB Liquid Additive -LA**			**2003**	**2003**	**2001**
	1	Nitrous Acid, Sodium Salt Solution (Sodium Nitrite)		**7632-00-0**	√	√	√
4)		**AB Z**			2004	2003	2001
	1	Phosphoric Acid		**7664-38-2**	√	X	N/APP
	2	Nitric Acid		**7897-37-2**	√	X	N/APP
	3	Zinc Oxide		**1314-13-2**	√	X	N/APP
5)		**Makeup A**			2002	2003	2001
	1	Phosphoric Acid		**7664-38-2**	√	√	N/APP
	2	Zinc Oxide		**1314-13-2**	√	√	N/APP
	3	Manganese DI-Oxide/Manganese Monoxide		**001313-13-9**	√	√	N/APP
	4	Nickel (II) Nitrate (NI(No3)2)		**13138-45-9**	√	√	N/APP
	5	Sodium Hydroxide		**001310-73-2**	√	√	N/APP
	6	Nitric Acid (Zinc Nitrate)		**7697-37-2**	√	√	N/APP
	7	Fluoride Compound, Inorganic, N.O.S.((NH4)HF2 Ammonium Fluoride)		**1341-49-7**	√	√	N/APP
6)		**Makeup B**			2003	2003	2001
	1	Sodium Nitrate		**007631994**	X	X	√
	2	Phosphoric acid		**7664-38-2**	√	√	√
	3	Nitric acid		**7697-37-2**	√	√	X
	4	Sodium Hydroxide		**1310-73-2**	√	√	X
	5	Caustic Potash/Potassium Hydroxide		**001310583**	√	√	X

√ indicates listing of the respective compounds in the site-specific or conceptual data documents is established
N/APP means the compound(s) was not listed in the data source inventory from the respective facility.
X indicate these chemicals were not listed in the specified facility documents

6.3.1 Discussion of Zinc Phosphate Product Composition Comparison

The main observations from the previous table:

1. The previous table illustrates how major differences can exist between the various sources of data. The degree of detail differs depending on the accessibility of information and what data can be readily communicated. The replenisher is an example of the differences between site specific and conceptual data products. Even though the same product name is used, its chemical composition can vary from site to site. The site-specific source data listed zinc oxide with CAS No. 001314-13-2 in its MSDS and NPRI documents, while conceptual data reported the use of zinc nitrate CAS No. 7779886 in the TRI document. Both are constituents in the replenisher used at both facilities, but are not consistently treated in terms of data reporting. These two compounds have different chemical abstract service numbers and thus different chemical constituents, which may later deliver inconsistent information as each CAS number delivers specific information about the product's physical, chemical, safety and health hazards data.
2. Waste nitrates are typically a substance of concern but site specific constituents records do not indicate or suggest their presence in some products such as the replenisher, but there is the possibility that zinc nitrate would form during the process. This formation would only occur, however, under precise conditions and thus does not accidentally form easily (Webelements, 2004). Thus, it may appear that the site specific process is more environmentally benign compared to the conceptual database, which does list nitrate compounds to begin with.

3. Similarly, manganese monoxide with (CAS No. 1344-43-0) is listed in the MSDS and NPRI documents from the site specific source, while manganese phosphate with (CAS No. 18718-07-5) is reported from conceptual TRI documents. Again, both are constituents in the replenisher, but the listings differ. As with the waste nitrates, if phosphorous compounds are regulated, it will appear as if site-specific processes may be more environmentally benign because such substances are not listed but may later form during process reactions. While it can be argued that emissions testing may pick up such newly formed substances later, they would not have been listed at the outset. Ironically, using conceptual data may pick up on this compound and thus suggests a situation where using site specific data would have been less conservative and even perhaps erroneous! This can confuse LCA users who are evaluating impact amounts due to certain compounds in an industrial process, or who are required to regulate the waste effluent compounds of a process, where it is apparent that facilities use different compounds under the same product name. General conclusions about a process should be used with caution.
4. Other products, for example makeup A that contains nickel, was only reported from Facility A, so LCA practitioners may assume that Facility B does not use it, that it is not regulated, or falls below a threshold criteria for measurement.
5. Within the replenisher some chemical compounds, such as ammonium fluoride are only reported from the site specific MSDS and NPRI documents. This may be partly explained due to the specifics of the zinc phosphate stage at this facility because different types of metal were added to the vehicle's BIW which may require some adjustments to the process chemistry. Although these are applied at

small concentrations, their total amount is significant in the stage under consideration. This is another challenge for using conceptual LCI data or using several inconsistent sources because unique (i.e., site specific) parameters or conditions might be missed.

6. In comparing the list of compounds, for example within the replenisher, only two out of the seven compounds listed are reported in both sources: phosphoric acid and nickel nitrate. The remaining compounds (eg. manganese phosphate and manganese monoxide) may be equivalent in function to some other products at the site specific facility but this would require expert confirmation. Under the same product name, several different compounds may be used in various facilities because of facility specific operations and technology. A similar discussion could be made for other compounds such as Makeup B.
7. Both surrogate and site specific facilities did not include the percentage of city water versus de-ionized water used in each product. It is important to include such basic material consumption information as part of any inventory.

Interestingly, some compounds such as AB FSA were absent from the TRI and NPRI documents despite being identified in the basic process flowcharts of Facility A which may indicate that they are used in amount smaller than the threshold reporting amounts. This can be a significant disadvantage if an LCI exercise depended on conceptual based data sources alone because the available information is clearly incomplete. Furthermore, during the thesis research, the conceptual data documents were provided first. Although they proved a useful starting point, it was only after the site specific data was received that it became apparent the potential amount of significant information could be missing.

6.4 Effect of Different Concentrations of Products Constituents in g/veh

The table below shows the percentage difference between the two data sources from the two facilities, and the effects on the concentrations of selected compounds and their total usage amounts expressed in the functional unit g/vehicle.

Table 10: Amounts of compound used based on two site-specific sources, and conceptual TRI in (g/veh)

S/No.	*Product/ Chemical Compound*	Concentration				Prod/Cmpd. Usage Amount in (Lbs)			Usage Amount in (g/vehicle)			(i) Diff of (3)-(1) g/veh	(ii) Diff of (3)-(2) g/veh	(iii) Diff. of (1)-(2) g/veh	% Difference (A)	% Difference (B)	% Difference (C)
		Facility A MSDS doc.	Facility A MSDS Avg Conc.	Facility A NPRI doc.	Facility B Avg	Facility A MSDS Avg. Conc.	Facility A NPRI Avg. Conc.	Facility B TRI	Facility A MSDS doc. (1)	Facility A NPRI doc. (2)	Facility B (3)						
	Replenisher					847422	868608	577200	1566	1372	1166						
1	Phosphoric Acid	30-60	45.0	27.5	7.5	381340	238867	43290	705	377	88	-617	-290	327.3	-88	-77	46
2	Zinc Nitrate				5			28860			58						
2	Zinc Oxide	5-10	7.5	7.5		63557	65146		117	103				14.5			12
3	Manganese Phosphate				7.5			43290			88						
3	Manganese Monoxide	1-5	3.0	3.0		25423	26058		47	41				5.8			12
4	Nickel Nitrate	1-5	3.0	3.0	5	25423	26058	28860	47	41	58	11.3	17	5.8	19	29	12
5	Zinc Dihydrogen Phosphate				12.5			72150			146						
6	Ammonium Fluoride	1-5	3.0	1.0		25423	8686		47	14				33.3			71
7	Nitric Acid	1-5	3.0	3.0		25423	26058		47	40				6.8			15

6.4.1 Discussion of Concentration Percentage Comparison Using g/vehicle

There are notable reporting discrepancies. For example, the phosphoric acid concentration mean was reported to be of 7.5% from conceptual data, 45% using Facility A MSDS documents, and 27.5% from the Facility A NPRI reports. This illustrates how variable sources have contradictory information and emphasizes the need to have comprehensive background information and possibly general knowledge of the site specific facility or process in order to properly select the concentration to be used in an LCA study. As can be seen, 7.5% appears too low of a concentration compared to the 27.5% or the 45%, but there is no definitive method for knowing in advance what surrogate concentration would have been acceptable. Overestimating or underestimating values is a very real possibility.

Nickel, from the nickel nitrate compound, is one of the heavy metals used in the pretreatment process in addition to manganese and zinc. They are harmful to the environment (PF Online, 2004) and are regulated. While their concentration in this study may be relatively small compared to other compounds, a small difference in the conceptual versus site specific data can lead to significant overall differences. For example, the Facility B TRI average concentration for nickel nitrate is reported as 5%, while Facility A's two references used 3%. If the mean concentration from Facility B TRI is used, it would result in an amount greater than the amount used in Facility A by 19% to 29%. Effects from heavy metals represent a category of impacts in which even small amounts can have disproportionately large impacts (Graedel, 2002).

The percent difference in amounts of the products reported using g/vehicle in Table 10 between Facility B and Facility A MSDS documents ranges from 19% to 88%, and between Facility B and Facility A government reports ranges from 29% to 77%. The difference between the two site-specific sources ranges from 12% to 71%. There can be surprising and significant inconsistencies among the sources despite reporting similarities.

6.5 Comparison of the Concentration Difference between the Two Data Inventories in g/m^2

The following table shows the percentage difference between the two facilities sources calculated using the functional unit g/m^2.

Table 11: Amount of compounds used based on two site-specific (Facility A) documents, and the conceptual (Facility B) TRI documents (g/m^2)

		Concentration				Prod/Cmpd. Usage Amount in (Lbs)			Usage Amount in (g/m2)			(i) Diff of (3)-(1) g/m2	(ii) Diff of (3)-(2) g/m2	(iii) Diff of (1)-(2) g/m2	% Difference (i)	% Difference (ii)	% Difference (C)
S/No.	*Product/Constituents Name*	Facility A MSDS doc.	Facility A MSDS Avg Conc.	Facility A NPRI doc.	Facility B Avg. Conc.	Facility A MSDS amount	Facility A NPRI Avg. Conc.	Facility B TRI	Facility A MSDS doc. (1)	Facility A NPRI doc. (2)	Facility B (3)						
Replenisher					X	847422	868608	577200	10.6	10.84	11.67						
1	Phosphoric Acid	30-60	45.0	27.5	7.5	381,340	238,867	43290	4.86	2.98	0.88	-3.89	-2.11	1.78	-82	-71	37
2	Zinc Nitrate (ZN(NO3)2				5			28860			0.58						
2	Zinc Oxide	5-10	7.5	7.5		63,557	65,146		0.79	0.81				-0.02			-2
3	/Manganese Phosphate				7.5			43290			0.88						
3	Manganese Monoxide	1-5	3.0	3.0		25,423	26,058		0.32	0.33				-0.01			-2
4	Nickel Nitrate Ni(NO3)2	1-5	3.0	3.0	5	25,423	26,058	28860	0.32	0.33	0.58	0.27	0.26	-0.01	46	44	-2
5	Zinc Dihydrogen Phosphate (ZN(H_2PO_4)$_2$)				12.5		0	72150			1.46						
6	Ammonium Fluoride ((NH4)(HF2))(Complexed Fluoride)	1-5	3.0	1.0		25,423	8,686		0.32	0.11				0.21			66
10	Nitric Acid	1-5	3.0	3.0		25,423	26,058		0.32	0.33				-0.01			-2

6.5.1 Discussion of Concentration Comparisons in g/m²

1. The differences in the results are similar to those discussed for Table 10, except that a new functional unit is used.
2. The percentage difference that was calculated for some constituents between the two data sources varies considerably from more than 46% up to 82%.

6.6 Comparison of the reportable compounds usage amounts

The waste annual reports from the two facilities follow the format required by government regulations in the two countries. Both emissions inventories (NPRI and TRI) use similar nomenclature and structure. These reports include flowcharts with the initial usage amounts of the regulated compounds such as zinc, manganese and nickel and their discharge in a wastewater form or as solid waste form. besides that these flowcharts include other portions and amounts described as either adhered to the metal or reported as losses or non-reportable amounts. The differences arising from using the two different emissions reports related to the zinc phosphate stage emission data will be analyzed in Table 12.

Table 12: Comparison of total compound usage amounts as found in NPRI/TRI documents process flows

Facility	Reportable compound	Chemical Name	Product Name / Product Use	Amount of Product Used (g)	Total Quantity of Product Used for All Parts			Quantity of Compound used for all parts	Total Quantity of Compound Used for All Parts		
					Total Amount of Product Used (g)	g/veh	g/m2	Compound Wt. [g]	g	g/veh	g/m2
Facility B	Manganese (& its compounds)	Manganese Phosphate	Replenisher	261,812,148	261,812,148	1166	10.05	19,635,911	19,635,911	87.47	0.75
Facility A		Manganese Monoxide	Replenisher	393,991,903				11,820,000			
		Manganese DI-oxide	Makeup A	374,212	394,366,114	1373	9.25	28,000	11,848,000	41.26	0.28
Difference of Facility A-Facility B			2 products are used in Facility A		132,553,966	207	-0.8		-7,787,911	-46.2	-0.48
Percentage Difference					**34**	**15**	**-8**		**-40**	**-53**	**-63**
Facility B	Zinc (& its Compounds)	Zinc Dihydrogen Phosphate	Replenisher	261,812,148	261,812,148	1166	10.05	32,726,519			
		Zinc Nitrate	Replenisher	261,812,148	261,812,148	1166	10.05	13,090,607	45,817,126	204.09	1.76
Facility A		Zinc Oxide	Makeup A	374,212				11,000			
			Replenisher	393,991,903	394,366,114	1373	9.25	29,550,000	29,561,000	102.95	0.69
Difference of Facility A-Facility B			2 products are used in Facility A		132,553,966	207	-0.8		-16,256,126	-101	-1.07
Percentage Difference					**34**	**15**	**-8**		**-35**	**-50**	**-61**
Facility B		Nickel Nitrate	Replenisher	261,812,148	261,812,148	1166.2	10.05	13,090,607	13,090,607	58.31	0.72
Facility A		Nickel Nitrate	Makeup A	374,212				19,000			

	Nickel Compounds		Replenisher	393,991,903	394,366,114	1373	9.25	11,820,000	11,839,000	41.23	0.28
Difference between Facility A & Facility B			2 products are used in Facility A		132,553,966	207	-0.8		-1,251,607	-17	-0.44
Percentage Difference					**34**	**15**	**-8**		**-10**	**-29**	**-61**
Facility B	**Nitrate compounds**	Nickel Nitrate	Replenisher	261,812,148	261,812,148	1166	10.05	13,090,607			
		Zinc Nitrate	Replenisher	261,812,148	261,812,148	1166	10.05	13,090,607	26,181,215	116.62	1.01
Facility A		Nickel Nitrate	Makeup A	374,212				19,000			
			Replenisher	393,991,903	394,366,114	1373	9.25	11,820,000	11,839,000	41.23	0.28
Difference between Facility A & Facility B			2 products are used in Facility A		132,553,966	207	-0.8		-14,342,215	-75	-0.73
Percentage Difference					**34**	**15**	**-8**		**-55**	**-65**	**-72**
Facility B	**Sodium nitrite**	Sodium nitrite	Liquid Additives	27,596,416	27,596,416	122	1.06	11,728,477	11,728,477	52.24	0.45
Facility A		Sodium nitrite	Liquid Additives	37,448,390	37,448,390	130	0.88	10,298,000	10,298,000	35.87	0.24
Difference between Facility A & Facility B					9,851,975	8	-0.18		-1,430,477	-16	0
Percentage Difference					**26**	**6**	**-17**		**-12**	**-31**	**-46**
Facility B	**Nitric acid**	Nitric acid	Liquid Additives	319,781	319,781	1.42	0.01	24,040	24,040	0.11	0
Facility A		Nitric acid	Makeup A	374,212				11,000			
			Makeup B	7,044,253				211,000			
			Replenisher	393,991,903	401,410,367	1398	9.42	11,820,000	12,042,000	41.94	0.28
Difference between Facility A & Facility B			3 products are used in Facility A		401,090,586	1397	9.4		12,017,960	42	0.28
Percentage Difference					**100**	**100**	**100**		**100**	**100**	**100**

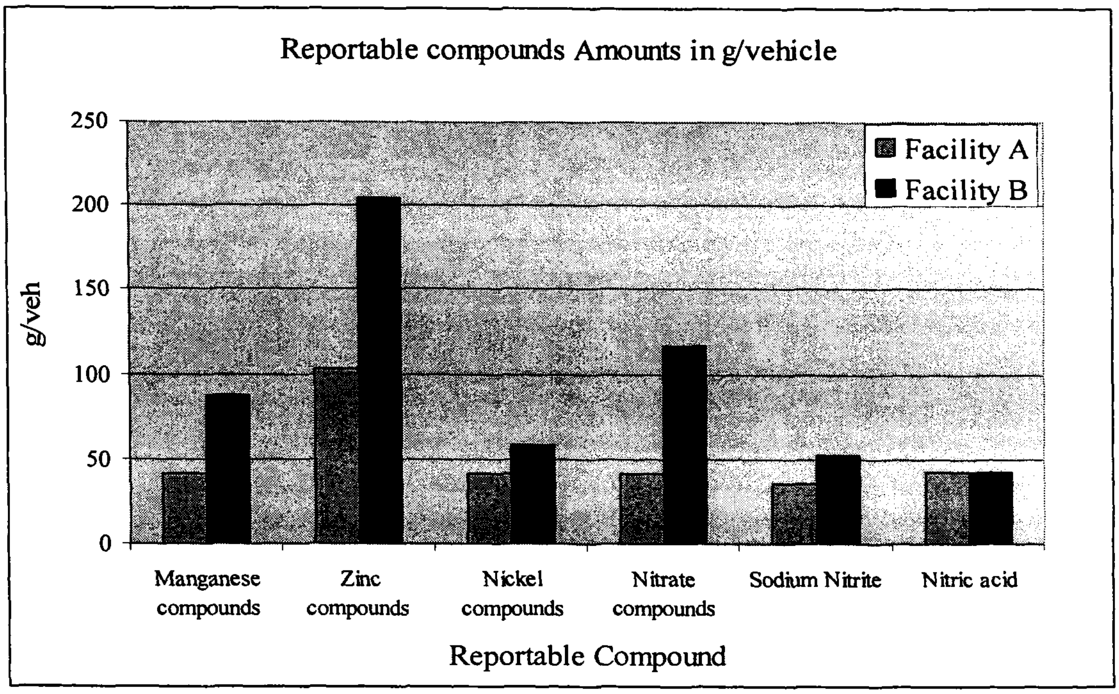


Figure 9: Comparison of reportable compounds amount in g/veh using Facility A site-specific NPRI records vs. Conceptual Facility B TRI reports as shown in Table 12

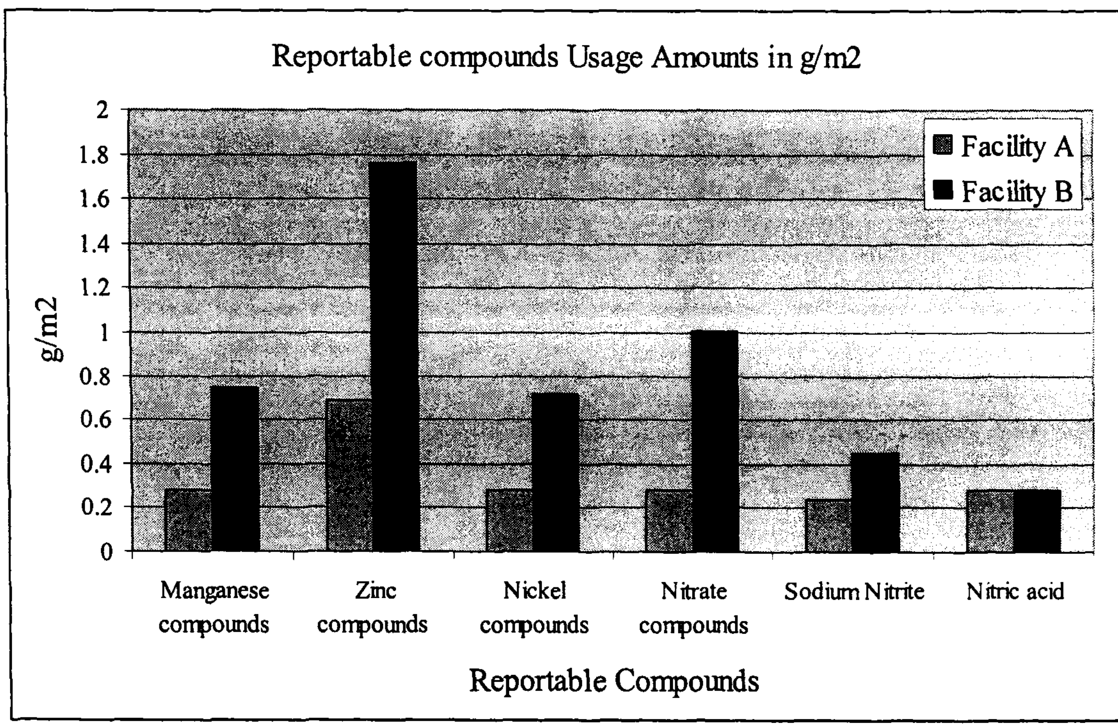


Figure 10: Comparison of reportable compounds usage amounts in g/m^2 using Facility A NPRI documents and Facility B TRI documents as shown in Table 12

6.6.1 Discussion of Comparison based on TRI and NPRI Documentation

When comparing the total amount of products used between the two data sets, Facility A uses greater amounts in g/veh. However, if g/m^2 is used this conclusion is reversed and Facility B used greater amounts than Facility A which is indicated by negative percent difference with the exception of the nitric acid compounds.

When comparing compounds, whether in g/veh or g/m2 units, site-specific data at Facility A indicates that it uses lower amounts of the regulated compounds amounts than the conceptual source at Facility B except for the nitric acid compound. The consumption of larger amount of product should not always be interpreted as higher amounts of hazardous materials used as well.

6.7 Summary tables and emissions amounts

The amounts of wastewater and sludge reported in the conceptual data and site specific data are compared in Table 13 below. Air emissions appear to be negligible. Part of the compounds are adhered to the metal on (BIW) and there are portion of the compounds noted as non-reportable. An overall mass balance on these heavy metals is shown.

Table 13: Mass balance including selective waste effluent for the heavy metal amounts using the facilities emissions reports of the zinc phosphating stage in grams

Facility Name	Reportable category	FATE FLOW								Remaining Balance of compound
		Compound amount				Waste Effluent				
		Compound Name	Quantity of Compound Used (g)	Total quantity of compound used for all parts (g)	On BIW	Waste-water	Land (sludge)	Air	Non Reportable	
					g					
Facility B	**Manganese (& its compounds)**	Manganese Phosphate	19,635,911	19,635,911	4934606	171457	1943180	0	12586669	0
		Manganese Monoxide	28,000							
Facility A		Manganese Dioxide	11,820,000	11,848,000	4678000	824000	3670000	0	2676000	0
	Difference of Facility A-Facility B			-7,787,911	-256605.61	652543	1726820	0	-9910669	
	Percentage Difference			**-40**	**-5**	**79**	**47**		**-79**	

		Zinc Dihydrogen Phosphate	32,726,519							
Facility B	**Zinc (& its compounds)**	Zinc Nitrate	13,090,607	45,817,126	13287012	253103	5441266	0	26835745	0
		Zinc Oxide	11,000		16884000	790000	6062000	0	5824000	
Facility A		Zinc Oxide	29,550,000	29,561,000	16884000	790000	6062000	0	5824000	1,000
	Difference of Facility A-Facility B			-16,256,126	3,596,988	536,897	620,734	0	-21,011,745	
	Percentage Difference			**-35**	**21**	**68**	**10**		**-78**	
Facility B		Nickel Nitrate	13,090,607	13,090,607	2941531	111130	1149851	0	8888550	-454
	Nickel Compounds	Nickel Nitrate	19,000							
Facility A		Nickel Nitrate	11,820,000	11,839,000						
	Difference of Facility A-Facility B			-1,251,607						
	Percentage Difference			**-10**						

Table 14: Selective waste effluent for the heavy metal amounts using the facilities emissions reports of the zinc phosphating stage in g/vehicle

Facility Name	Reportable category	*Fates (using wastes flows from Facility A & Facility B)*			FATE FLOW				
		Compound Name	Quantity of Compound Used (g)	Total quantity of compound g/veh	Waste Effluent: On BIW (g/veh)	Waste Effluent: Waste-water (g/veh)	Waste Effluent: Land (sludge) (g/veh)	Waste Effluent: Air (g/veh)	Non Reportable (g/veh)
Facility B	**Manganese (& its compounds)**	Manganese Phosphate	19,635,911	87	22	0.76	8.66	0	56
Facility A		Manganese Monoxide	28,000						
		Manganese Dioxide	11,820,000	41	16	2.87	12.78	0	9.3
	Difference of Facility A-Facility B			-46	-6	2	4.13	0	-46
	Percentage Difference			**-53**	**-26**	**73**	**32**		**-83**
Facility B	**Zinc (& its compounds)**	Zinc Dihydrogen Phosphate	32,726,519						
		Zinc Nitrate	13,090,607	204	59	1.13	24.24	0	119
Facility A		Zinc Oxide	11,000				21.11	0	20
		Zinc Oxide	29,550,000	103	59	2.75	21.11	0	20
	Difference of Facility A-Facility B			-101	0	1.624	-3.125	0	
	Percentage Difference			**-50**	**-1**	**59**	**-13**		

Facility B	**Nickel Compounds**	Nickel Nitrate	13,090,607	58	13	0.50	5.12	0	
		Nickel Nitrate	19,000						
Facility A		Nickel Nitrate	11,820,000	41	**Waste effluent Fates Not Available**				
	Difference of Facility A-Facility B			-17					
	Percentage Difference			**-29**					

Table 15: Selective waste effluent for the heavy metal amounts at both data sets of the zinc phosphating stage in g/m²

Fates (using process flows from Facility A & Facility B)					FATE FLOW				
Facility Name	**Reportables category**	**Compound Name**	**Quantity of Compound Used**	**Quantity Used**	**On BIW**	**Wastewater**	**Land (sludge)**	**Air**	**Non Reportable**
			g	**g/m²**					
Facility B	**Manganese (& its compounds)**	Manganese Phosphate	19,635,911	0.75	0.189	0.007	0.075	0	0.483
Facility A		Manganese Monoxide	28,000						
		Manganese DI-oxide	11,820,000	0.28	0.110	0.019	0.086	0	0.063
	Difference of Facility A-Facility B			-0.48	-0.08	0.01	0.01	0	-0.42
	Percentage Difference			**-63**	**-42**	**66**	**13**		**-87**
Facility B	**Zinc (& its Compounds)**	Zinc Dihydrogen Phosphate	32,726,519						
		Zinc Nitrate	13,090,607	1.76	0.510	0.010	0.209	0	1.030
Facility A		Zinc Oxide	11,000					0	
		Zinc Oxide	29,550,000	0.69	0.396	0.019	0.142	0	0.137
	Difference of Facility A-Facility B			-1.07	-0.11	0.01	-0.07	0	-0.89
	Percentage Difference			**-61**	**-22**	**48**	**-32**		**-87**

Facility B		Nickel Nitrate	13,090,607	0.50	0.113	0.004	0.044	0	
Facility A	**Nickel Compounds**	Nickel Nitrate	19,000						
Facility A		Nickel Nitrate	11,820,000	0.28	0.278				
Difference of Facility A-Facility B			-1,251,607	-0.22	0.165				
	Percentage Difference		**-10**	**-45**	**59**				

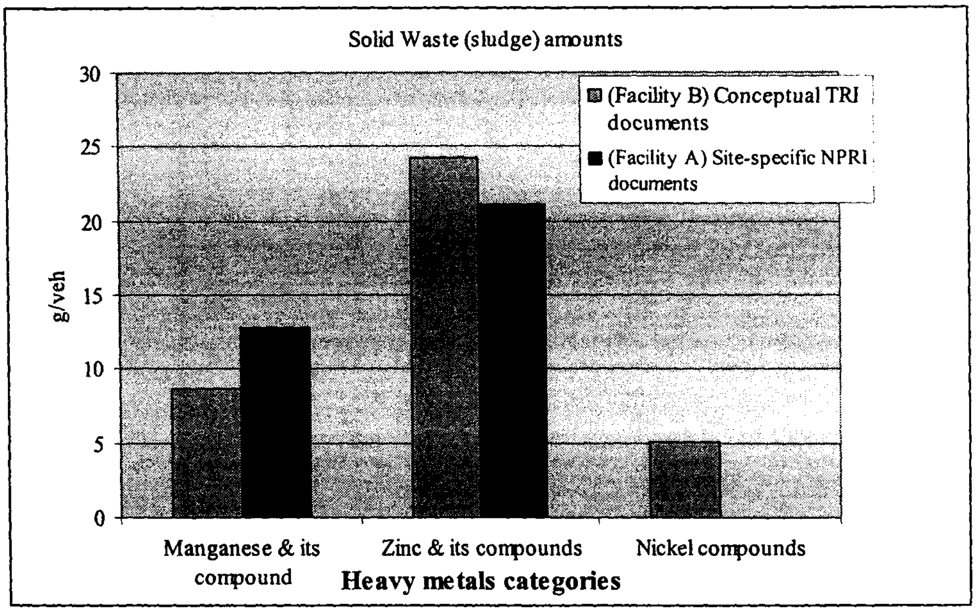


Figure 11: Comparison of reportable heavy metals discharged from both facilities as solid waste in g/veh using site-specific NPRI reports vs. Conceptual TRI reports as shown in Table 14

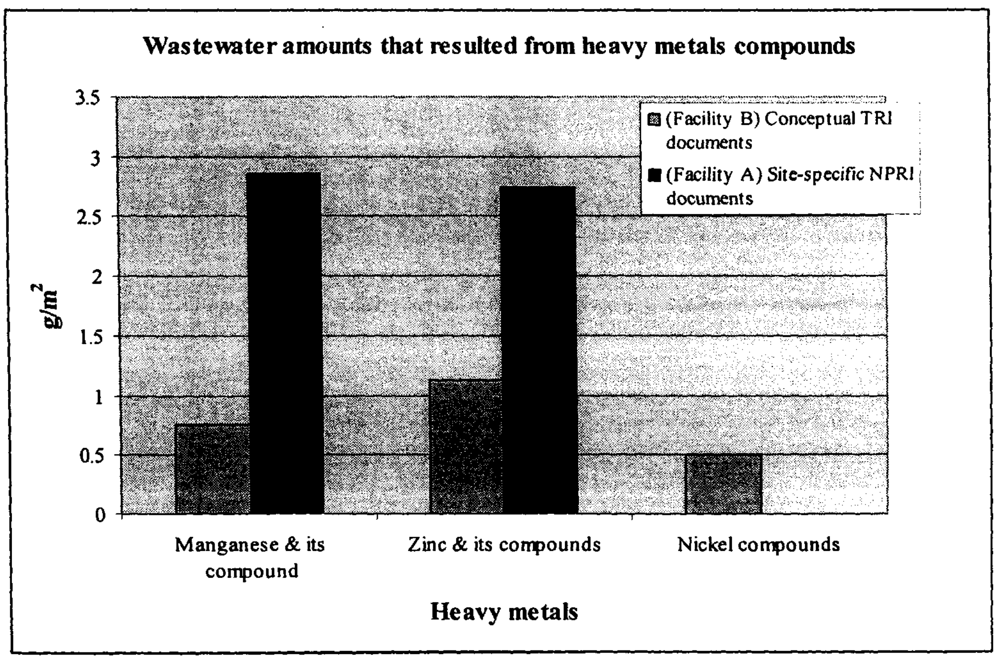


Figure 12: Comparison of reportable heavy metals discharged from both facilities as wastewater in g/m^2 using site-specific NPRI reports vs. Conceptual TRI reports as shown in Table 15

6.7.1 Emissions and mass balance calculations on the heavy metals category

The key observations from the previous table are:

1. Different facilities produce variable amounts of sludge and wastewater. Although the g/m^2 functional unit would appear to be more preferable unit for LCA studies that involved such processes, in this study the g/veh functional unit may be more reliable because the number of vehicles pretreated were based on a verified expert estimate or a reviewed literature source. Surface area values as explained earlier came from much more disparate sources.
2. Facility B at the surrogate source uses more heavy metals compounds as inputs than Facility A as shown in Figures 9 and 10 however, the wastewater effluent due to these compounds from Facility A is greater in g/veh units as well as in g/m^2 units than Facility B, see Tables 14 and 15.
3. As for the sludge percentage difference it varies where Facility A discharge more manganese solid waste than Facility B but it generates lesser zinc solid waste than the conceptual site at Facility B, in both functional units.
4. Comparing nickel wastewater amounts and solid waste was not possible as no discharge flows are provided from Facility A for this compound.
5. The zinc and nickel compounds have a remaining balance difference of 1000g and 454 g respectively, which may be due to the rounding off of values: the difference is not considered significant when compared to the much larger overall amounts.

6.8 Sensitivity analysis

A sensitivity analysis can demonstrate where variations in the data will most affect the LCI results. The sensitivity analysis will test for the effect of surface area and vehicle production on the replenisher and liquid additive because other compounds had inconsistently or incompletely reported data.

The data available from conceptual sources has been compiled and summarized in Table 16 below, which shows the usage amounts of the replenisher and liquid additive expressed in g/m^2.

Table 16: Effect of variable conceptual data vehicle surface area and production volume data on the replenisher and liquid additives usage amounts in (g/m^2)

		Conceptual Surface Areas		
Vehicle Production	**Total usage from TRI (lbs)**	**Surface area (m^2)**	**Surface area (m^2)**	**Surface area (m^2)**
		79	**102**	**116**
		Replenisher usage amount in g/m^2		
200000	577200	16.6	12.8	11.3
224500	577200	14.8	11.4	10.1
249000	577200	13.3	10.3	9.1
		Liquid additive usage amount in g/m^2		
200000	60480	1.7	1.3	1.2
224500	60480	1.5	1.2	1.1
249000	60480	1.4	1.1	0.9

The average surface area, or 148 m^2, from both the V1 and V2 vehicle models produced at Facility A will be assumed to represent the actual or absolute surface area of a vehicle subjected to the pretreatment process for the purposes of this sensitivity analysis. Compared to the conceptual surface areas, the greatest difference is 47%; the range of surface area differences within the conceptual areas that an LCI practitioner would likely choose from is 25%, as shown in Table 17.

Table 17: Range in absolute and relative surface area differences among conceptual data and compared to site specific data.

Conceptual Surface Areas			*Site Specific*
Surface area (m^2)	**Surface area (m^2)**	**Surface area (m^2)**	**Surface area (m^2)**
79	102	116	148
Difference compared to site specific surface area			
-47%	-31%	-22%	0%
Range in conceptual area differences			
25%			

Similarly, the average vehicle production (245472 vehicles) from the site specific data (Facility A) will be assumed to be the actual or absolute vehicle production for comparing the conceptual production numbers. As shown in Table 18, the differences are less pronounced: there is a maximum 19% difference between conceptual and site specific data, and a difference of 20% within conceptual data sources.

Table 18: Range in absolute and relative vehicle production numbers among conceptual data and compared to site specific data.

Conceptual Vehicle Production			*Site Specific*
Veh Production	**Veh Production**	**Veh Production**	**Veh Prod**
200000	224500	249000	245472
Difference compared to site specific surface area			
-19%	-9%	1%	0%
Range in conceptual area differences			
20%			

To determine the effects of varying surface area and vehicle production values on the g/m^2 values of the replenisher and liquid additive, two values are assumed fixed from the site specific (Facility A) data:

1. An average replenisher usage amount of 10.6 g/m^2; and

2. An average liquid additive usage amount of 1.1 g/m^2.

These are then subtracted from each of the corresponding items in Table 16 and the percent differences as compared to the site specific values are given in Table 19. Reading across the rows gives the variation in usage amounts due to different surface areas for any particular production volume, while reading down the columns gives the variation in usage amounts due to different vehicle production volumes for any particular surface area.

Table 19: Range in differences between conceptual and site specific data using conceptual data for surface areas and vehicle production.

Vehicle Production	Total usage from TRI (lbs)	*Conceptual Surface Areas* Surface area (m^2)	Surface area (m^2)	Surface area (m^2)	
		79	**102**	**116**	***Range in diff due to area***
Difference in replenisher usage amount in g/m^2 compared to site specific 10.6 g/m^2					
200000	577200	57%	21%	7%	50%
224500	577200	40%	8%	-5%	44%
249000	577200	25%	-3%	-14%	40%
	Range in diff due to veh production	31%	24%	21%	
Difference in liquid additive usage amount in g/m^2 compared to site specific 1.1 g/m^2					***Range in diff due to area***
200000	60480	55%	18%	9%	45%
224500	60480	36%	9%	0%	36%
249000	60480	27%	0%	-18%	45%
	Range in diff due to veh production	27%	18%	27%	

Comparing Tables 17 and 18 against Table 19 leads to the following observations:

- A difference in conceptual surface areas of 25% - representing the range of readily available data - results in usage range variations of 40% to 50% for the replenisher, and 36% to 45% for the liquid additive.

- A difference in conceptual vehicle production volumes of 20% - again representing the range of readily available data - results in usage range variations of 21% to 31% for the replenisher, and 18% to 27% for the liquid additive.

Thus, based on this limited data set, it appears that changes in vehicle production volumes used for estimating LCI amounts will lead to an approximately similar magnitude of change in the usage amounts, whereas a change in the surface areas could result in 1.5 to 2 times as much change in the estimated usage amounts. Arguably, the greater the data quality and confidence behind the surface area estimate, the more credible the final results.

6.9 Comparison of Multiple Conceptual Data Sources

This section examines the differences that potentially exist if several data sources are available for the same product or compound. In particular, the focus will be on MSDS documents which would be one of the literature sources readily available to LCA practitioners.

Table 20: Comparing selective products as an example of the differences exist among several sources

	Product Name/Chemical Compound	CAS. No.	Sources of CAS. No.						Concentration /Conc. Range					
			Facility A NPRI Doc.	Detailed MSDS	Facility A MSDS	Corporate MSDS	Facility B TRI	Online MSDS	Facility A NPRI Doc.	Detailed MSDS	Facility A MSDS	Corporate MSDS	Facility B TRI	Online MSDS
Replenisher														
1	Phosphoric Acid	7664382	√	√	√	√	√	√	27.5	5-10	30-60	10-30	7.5	15-40
2	Zinc Nitrate (ZN(NO3)2)	7779886		√			√			1-<5/1-2			5	
2	Zinc Oxide	001314-13-2	√		√	√		√	3		5-10	5-10		5-10
3	Maganese Phosphate	18718-07-5		√			10124546			10-<20/10-15			7.5	
3	Manganese Monoxide	1344-43-0	√		√	√		√	3		1-5	1-5		1-5
4	Nickel Nitrate Ni(NO3)	013138459	√	√	√	√	√	√	3	1-<5/1-2	1-5	1-5	5	1-5
5	Zinc Dihydrogen Phosphate	13598373		√			√			10-15			12.5	
6	Ammonium Flouride	001341-49-7	√		√			√	1		1-5			0.5-1.5
7	Potassium Hydrogen Diflouride	7789-29-9		√		7789233				1-<5/1-2		1-5		
8	Deionzied Water	7732-18-5		√						2-5				
9	Tap Water (Potable)	7732-18-5		√						60-65				
10	Nitric Acid	007697-37-2	√		√	√		√	3		1-5			1-5

6.9.1 Discussion of Comparison of Multiple Conceptual Data Sources

There are discrepancies between all MSDS data sources. Different sources use different chemical compounds as well as different CAS numbers for a compound with synonyms, but in general most of the constituents are common.

Interestingly, the readily available, "general" online MSDS documentation for this research most closely matches the site specific facility's MSDS data. This suggests that online sources may be a reliable information source. For example, the phosphoric acid concentration at the site-specific sources ranges from 30% to 60%, but the site-specific NPRI denoted a concentration of 27.5%. Another example is the ammonium fluoride compound which was only mentioned in site-specific documents and in the online sources, not by corporate or suppliers but its concentration was different. As a result, there can be significant data gaps when using various MSDS or other similar documentation.

6.10 Data Quality Management of Selected Products Used in the Zinc Phosphate Stage

Table 21 shows the results of the data quality analysis by applying the remaining two indicators, reliability and completeness to the materials input data of the zinc phosphate stage in the pretreatment process. *Reliability* relates to the data source, method of acquisition and verification, and is represented by the first value in the total score.

Completeness relates to statistical properties of the data, how representative is the sample, and if the data period is sufficiently long to even out fluctuations, and is represented by the second value. The remaining three values were previously scored in Chapter 5.

Table 21: Selective data quality indicators used in analyzing the zinc phosphate stage input inventories.

S/No.	Product Name	Reliability Score		Completeness		Comments	Total Score
		Site-specific	Conceptual	Site-specific	Conceptual		
1	**Replenisher**	1 Amount of input material is a verified data based on measurements	2 Non-verified data based on measurements	2 Representative data from a smaller number of sites but for adequate periods	4 Incomplete data from an adequate number of sites and periods	Facility B data lack MSDS documents which may explain and confirm the data found in the inventory provided by the plant	Facility A (1,2,1,1,1) Facility B (2,4,1,2,2)
2	**AB FSA**	5 Incomplete data or No data provided	5 Incomplete data or No data provided	4 Incomplete data from an adequate number of sites and periods	4 Incomplete data from an adequate number of sites and periods		Facility A (5,4,1,1,1) Facility B (5,4,1,2,2)
3	**Liquid Additive**	1 Amount of input material is a verified data based on measurement	2 Non-verified data based on measurements	2 Representative data from a smaller number of sites but for adequate periods	4 Incomplete data from an adequate number of sites and periods	Facility B data lack MSDS documents which may explain and confirm the data found in the inventory provided by the plant	Facility A (1,2,1,1,1) Facility B (2,4,1,2,2)
4	**AB Z**	5 Incomplete data or No data provided	5 Incomplete data or No data provided	5 Incomplete data from a smaller number of sites and/or from shorter periods	5 No data provided	MSDS was only provided from Facility A, but no usage amounts.	Facility A (5,5,1,1,1) Facility B (5,5,1,2,2)

5	**Makeup A**	5 Incomplete data or No data provided	5 Incomplete data or No data provided	5 Incomplete data from a smaller number of sites and/or from shorter periods	5 No data provided	MSDS was only provided from Facility A, but no usage amounts	Facility A (5,5,1,1,2) Facility B (5,5,1,2,1)
6	**Makeup B**	5 Incomplete data or No data provided	2 Non-verified data based on measurements	5 Incomplete data from a smaller number of sites and/or from shorter periods	4 Incomplete data from an adequate number of sites and periods	Facility B listed less chemical compounds in its inventory, and Facility A provided no total usage amount.	Facility A (5,5,1,1,2) Facility B (2,4,1,2,1)

6.10.1 Discussion on Data Quality Indicators

As can be seen from the previous table, the score of different products used in this stage varies from one facility data set to another. These variable indicators can identify weaknesses in the data in order to enhance the method and quality of data collection for other future studies. For example, Facility B's score with regard to the replenisher is (1,2,1,1,1) which can be classified as data of high quality in general because most scores are "1" and only weakness is the reliability of the data because of the lack of verification from site experts. In general, the data used in this research scored highly with respect to the temporal, geographical and technological aspects (see Chapter 5).

The pedigree matrix in this analysis suggests that most of the data quality and uncertainty issues are likely related to the first two indicators in the matrix: reliability and completeness reflected as a lack of data. This deficiency arises from the lack of "information exchange". It is difficult to check the actual method of data measurement for each reported number because of the enormous amounts of information involved in any industrial process. Also, obtaining dependable data from more than one site in reasonable time and effort is difficult. The importance of having a contact person with expertise in the process under consideration to expertly judge or comment on the process will likely improve the quality of the data.

Chapter 7: Conclusions & Recommendations

This chapter develops the overall conclusions from the multiple analyses and recommends how a conceptual LCI can be made more representative to a site specific LCI.

7.1 Conclusions Regarding Conceptual Data Usage

Differences between conceptual and site-specific data exist at all levels, in the products used, their amounts, the compounds and constituents as well as their concentrations, and emissions. However, this difference does not appear to be consistent and therefore it may not be possible to assign a single, uniform "correction factor" to conceptual LCIs.

Both data sets are workable for the circumstances they represent although there are differences in representing a specific situation. Any LCI could be made more accurate and manageable if there is better accessibility needed data. If a conceptual LCI is developed and used to assess a new design, process, or facility, it can at least provide estimates about the materials consumed and emissions produced within a "working" order of magnitude. In the examples in this research, such estimates could then be scaled to the appropriate level by, for example, the number of vehicles produced. However, this issue emphasizes the significance of the data that will be used in normalization of input and output values. In this case, the key normalizers are the area of the vehicle and the number of vehicles produced. Furthermore, the issue of data transformation illustrates the impacts of the choice of *functional unit* on the outcome values. As was demonstrated in the sensitivity analysis, the choice of variables can significantly affect the resulting values used in an LCI.

If site specific data is available such data will likely result in a much more credible LCI on a local or perhaps even regional level for a certain process or facility. Having the benefit of expert contact and review of all assumptions and calculations to complete data gaps and to verify the accuracy of the analysis would be a tremendous asset. However, using case specific results on a global scale should be done with great attention to variability among facilities, processes even within the same industry as seen in this study. Generalizing LCA conclusions of one facility to all similar industries, especially from a lay perspective is not recommended.

Finally, most of the differences observed during the analyses varied considerably between the conceptually derived data and the supposed true values from the site specific data. However, most were within an order of magnitude and in some cases, were within what could be considered reasonable percentage differences given all the variables that could influence the analysis. While much improvement can be made in many different aspects, from a broad LCA perspective, where a basic knowledge of the impacts due to any activity is helpful to any industry, this level of credibility may be sufficient depending on the study goal and objectives.

7.2 Recommendations

This research demonstrates that data flaws and data gaps exist, even with site specific data, and a tremendous volume of information would be needed to be collected and verified. In practice, this leaves LCA practitioners with little choice but to use conceptual data to fill the missing gaps to a reasonable LCI. Clearly, such LCI may not be decisive or credible for aiding decision making in certain circumstances. Much more rigorously documented databases for LCI relevant information from all industries – although not yet a foreseeable reality – would be a tremendous asset.

Conceptual data that is derived from a single source and then used for within an LCI may be acceptable depending on the project's objectives, but to arrive at more sound conclusions several sites should be included within the same geographical and temporal zone. The use of common reporting procedures will also help achieve efficient and effective results.

Data quality management issues must be included in LCA studies to indicate the source of the data, any biases, and how data flaws could be corrected. The pedigree matrix as shown in this thesis may prove effective in less complex situations, but may be too general in other situations and requires further refinement.

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Vita Auctoris

Faiza Abdulrahem was born in 1967 in Aden, Yemen. She graduated from the Faculty of Engineering at Aden University in 1993. From there she worked for five years in consulting firm in Aden before immigrating to Canada. In summer 2002, she joined the University of Windsor, Ontario where she recently defended her thesis research for the Master's degree in Environmental Engineering at the University of Windsor and hopes to graduate in Fall 2004.